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1976
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The views expressed in this report are those of the authors and do not necessarily reflect the view of the committee, the Transportation Research Board, the National Academy of Sciences, or the sponsors of the project.

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INTRODUCTION

John B. Chernisky, Federal Highway Administration and Secretary of the TRB Committee on Transportation and Air Quality

The National Environmental Policy Act (NEPA) requires the assessment of anticipated impacts on the environment for each major federal action. The vehicles that use transportation facilities emit pollutants into the atmosphere; therefore, these facilities have some impact on the quality of the air.

The Clean Air Act requires that maximum allowable concentrations of pollution be established on a health-effect basis and that each state develop a plan for implementing these standards. The Federal-Aid Highway Act requires certain actions to ensure that highways to be constructed are consistent with the state implementation plans referred to above. This includes predicting levels of pollution after a proposed highway or series of highways (transportation system) has been completed and put into use. These predictions are performed by modeling the pollution impact on the atmosphere.

Pollutants are divided into 2 classes: relatively inert and reactive.

The inert pollutants are emitted from sources such as industrial stacks and vehicular exhaust pipes. Because of the turbulence of the atmosphere and topography (both natural and man-made), the pollutants eventually become diffused into small harmless traces in the atmosphere. How fast this occurs depends on how much pollutant is emitted, how turbulent the atmospheric conditions are, and whether the terrain aids or impedes diffusion. How much of each of these factors exists and what their combined effect is are referred to as diffusion modeling of inert (or nonreactive) pollutants. Some level of sophistication is required in developing and using these models to ensure reasonable levels of confidence in the predictions.

Reactive pollutants have similar diffusion patterns. Although the turbulence of the atmosphere affects their intermixing, chemical reactions occur among the gaseous particles. To model reactive pollutant behavior, one must consider, in addition to emissions, turbulence, and topography, the amount of sunlight, humidity, products of chemical reactions, and speed (or slowness) of these reactions. Different geographic regions will have different mixtures of gases in the lower atmosphere.

Studies have been and are being conducted to add accuracy to these estimating techniques. There is agreement on many topics, but apparent inconsistencies exist in others.

During the development of these sciences, the assessment of air quality impacts from proposed highways continues to be a requirement. The U.S. Department of Transportation and state transportation agencies are frustrated from the apparently inconsistent bits of information from these evolving sciences. They continue to ask for better tools to help estimate the quality of the air after the highway facilities are put into service.

Therefore, the U.S. Department of Transportation and the U.S. Environmental Protection Agency felt that a conference was needed on the state of the art in modeling. The Transportation Research Board Committee on Transportation and Air Quality conducted the Conference on the State of the Art of Assessing Transportation-Related Air Quality Impacts, which brought together experts in these areas of chemistry, meteorology, and transportation. These people, who are working at advancing the frontier of understanding, were provided the opportunity to become aware of each other's problems.

Another conference objective was to bring up-to-date information to those who use this developing science. This Special Report, which contains the conference papers, fulfills that objective.

WORKSHOP 1

PHOTOCHEMICAL OXIDANT MODELS

ISSUES IN OXIDANT MODELING

Joel L. Horowitz, Office of Policy Analysis, U.S. Environmental Protection Agency

Since 1969 a variety of legal requirements have been established that make it necessary to forecast the effects of changes in transportation systems on atmospheric oxidant concentrations. Such forecasts are needed in connection with the environmental impact statements required by the National Environmental Policy Act, the state implementation plans required by the Clean Air Act, and the certification process carried out under the Federal-Aid Highway Act.

The development of legal requirements for oxidant forecasting has been accompanied by the development of numerous techniques that planners might use to predict the effects of transportation changes on oxidant concentrations. These techniques range in complexity from the almost trivial to the almost incomprehensible. Some of the techniques require minimal skills and data to use, but others require large quantities of data, sophisticated computing facilities, and highly skilled users. Moreover, the accuracy of all the techniques is known poorly, if at all. Given these factors, it is not surprising considerable uncertainty and confusion exist as to the technical procedures that should be used to forecast the oxidant impacts of transportation system changes.

The proliferation of oxidant forecasting techniques and the confusion surrounding their use reflect the extreme difficulty of modeling the relation between the emissions of air pollutants by motor vehicles and other sources and the concentrations of oxidant in the atmosphere. The principal reason for this difficulty is that oxidant is not emitted into the atmosphere by any emissions source. Rather, it is the product of chemical reactions in the atmosphere involving a wide variety of organic compounds and oxides of nitrogen. The organics and nitrogen oxides are emitted by motor vehicles, various industrial and commercial operations, and certain natural processes. In forecasting oxidant levels or changes in oxidant levels, one must consider not only atmospheric dispersion and transport, as must be done with any air pollutant, but also a complex set of chemical reactions.

One of the consequences of the involvement of atmospheric chemical reactions in oxidant formation is that it is not possible to state a priori whether oxidant concentrations will decrease if emissions of oxidant precursors (organic compounds and nitrogen oxides) decrease. In the case of an inert pollutant, such as carbon monoxide, a decrease in emissions is likely to cause a decrease in concentrations, other things being equal. However, under certain conditions decreasing either organic or nitrogen oxide emissions can cause oxidant concentrations to increase. This observation leads to what might be the most basic questions about oxidant control from the point of view of transportation planners and others responsible for formulating and implementing public policy options: What kinds of emissions should be reduced in order to reduce oxidant concentrations? Can it be said with reasonable confidence that reducing emissions of organics or nitrogen oxides or both in some suitable proportion will reduce oxidant concentrations?

These questions are addressed in the papers by Dimitriades and by Myrabo, Wilson, and Trijonis, who conclude that achieving the ambient air quality standard for oxidant in urban areas requires substantial reductions of emissions of hydrocarbons and other

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reactive organics in the source areas. The situation with respect to nitrogen oxide emissions is more delicate. In some urban areas reductions of nitrogen oxide emissions are needed to attain or maintain the ambient air quality standard for nitrogen dioxide. Moreover, reductions in urban area nitrogen oxide emissions may be needed to control oxidant concentrations in rural areas. However, excessive reduction of nitrogen oxide emissions may increase the difficulty of controlling urban oxidant concentrations.

The question of the directionality of oxidant changes leads to the problem of estimating the magnitudes of these changes. The papers in this report describe 4 techniques that might be used to estimate the changes in oxidant concentrations resulting from changes in precursor emissions:

1. Linear or nonlinear rollback methods, by Dimitriades and by Myrabo, Wilson, and Trijonis;
2. Smog chamber models, by Dimitriades;
3. Statistical models, by Myrabo, Wilson, and Trijonis; and
4. Diffusion models, by Demerjian and by Ranzieri and Shirley.

These techniques also are addressed by Seinfeld and Eschenroeder.

Rollback is the simplest of the 4 approaches and the one that has received the most widespread use to date. Its drawbacks are well known. These include failure to incorporate explicitly the effects of nitrogen oxide emissions, lack of spatial and temporal disaggregation, and lack of a clear statistical meaning.

Diffusion models are the most sophisticated of the various modeling approaches and provide the most detailed (and, presumably, most realistic) description of the oxidant formation and dispersion process. These models offer the possibility of providing spatially and temporally disaggregated descriptions of the relation between oxidant and its precursors. However, the models have not yet reached a stage of development and verification such that the authors of papers in this report would advise an agency that does not already have access to a diffusion model to go to the expense and difficulty of acquiring one. On the other hand, agencies that have access to diffusion models probably should use them, preferably in parallel with other techniques and in connection with a program to monitor their validity.

Even when the current developmental problems have been solved, the cost and difficulty of using diffusion models will prohibit their use in many situations. Thus, there will remain a need for modeling techniques that are simpler than diffusion models but more sophisticated (and, presumably, more accurate) than rollback methods. Smog chamber models and statistical models estimated from aerometric data or, possibly, from data obtained through numerical experiments with diffusion models offer promising approaches to fulfilling this need. Both modeling approaches can incorporate nitrogen oxide effects explicitly, and statistical models may be capable of achieving spatial disaggregation. Each of the approaches has certain problems, the most notable being that they are at relatively primitive stages of development and of unknown validity. However, they are sufficiently easy and inexpensive to use that the authors of papers in this report suggest that planning agencies consider making use of smog chamber and statistical methods in parallel with rollback methods and, when available, diffusion models. The widespread use of smog chamber and statistical models, in parallel with other models and in connection with programs to monitor their validity, is likely to be the best way to acquire the information needed to assess the value of these techniques.

All of the applications of models to date have been based on the assumption that oxidant concentrations in a region are attributable to precursor emissions in the same region. Recently, however, it has been discovered that oxidant can be transported over distances of at least 30 miles (48 km) and that high oxidant concentrations exist in rural areas. These findings lead to several significant questions for urban-based oxidant models and oxidant control strategies.

1. To what extent are elevated rural oxidant concentrations caused by natural

sources and, therefore, uncontrollable?

2. To what extent does rural oxidant, whatever its source, contribute to urban oxidant concentrations?

3. To what extent are urban areas polluting rural areas?

4. Do the rural oxidant and transport phenomena imply that oxidant modeling and control can be carried out meaningfully only on a multiregional or multistate basis?

These questions are addressed in the paper by Angus and Martinez, who conclude that elevated rural oxidant concentrations are attributable largely to man-made emission sources. However, it was suggested in the workshop that this conclusion may be premature and that there is a possibility of significant natural contribution. It was also suggested that, based on chemical considerations, the transport of oxidant from rural areas into urban areas may have relatively little effect on urban oxidant concentrations but that the transport of oxidant precursors from rural areas into urban areas may be capable of affecting urban oxidant levels. All the authors agree that more research is needed before a satisfactory understanding of rural oxidants and transport and their implications for urban oxidant control is achieved.

It is clear from the papers in this report that the field of oxidant modeling contains many ambiguities and few unqualified conclusions. However, it is also clear that a variety of potentially promising modeling approaches exist. It is likely that the validity and usefulness of these approaches cannot be determined until there has been widespread experience with them. I hope that the papers in this report encourage potential users of the modeling techniques to become users and, thereby, contribute to the needed experience.

ACKNOWLEDGMENT

The views expressed in this paper are those of the author and are not necessarily endorsed by the U.S. Environmental Protection Agency.

CHEMISTRY

Basil Dimitriades, Environmental Services Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina

The subject of this paper essentially involves the problem of relating oxidant air quality to emissions. And because, unlike carbon monoxide, oxidant is a secondary pollutant, the problem is doubly complex. It has all the complexities of the dispersion process plus the complexities of the chemical process in which the reactant pollutants are converted into oxidants. This paper examines the various methods now available to relate ambient oxidant to emissions, but first discusses briefly the chemical and physical mechanisms by which emissions are dispersed in the atmosphere, get transported, and react to form urban, suburban, and nonurban oxidant.

CHEMICAL MECHANISM

Figure 1 shows the chemical process that occurs when hydrocarbon (HC) and nitrogen oxides (NO_x) in air are irradiated by sunlight. The overall process consists of 2 stages. In the first stage, NO is converted into NO_2; when all NO has reacted, O_3 begins to form and accumulate until either the irradiation ceases or the system runs out of reactants. This process was studied intensively in the laboratory (smog chambers), and the findings are as follows (1):

1. Increasing HC reactant concentration increases the rate of NO oxidation and in most cases increases resultant O_3 levels also (Figure 2);
2. Increasing NO concentration has a nonmonotonic effect, first increasing O_3 yield and then causing a decrease (Figure 3);
3. The nature of the HC reactant is also a factor; and
4. All these factors, HC, NO, irradiation time, and HC nature, interact to create further complications.

Subsequent mechanistic studies explained all these effects, at least for some hydrocarbons, e.g., propylene, n-butane. Thus, in a condensed form such a mechanism is approximately as follows:

$$NO_2 \xrightarrow{h\nu} NO + O \tag{1}$$

$$O + O_2 \xrightarrow{M} O_3 \tag{2}$$

$$O_3 + NO \rightarrow NO_2 + O_2 \tag{3}$$

$$O, O_3 + HC \rightarrow \text{products} + R \text{ (e.g., } R, RO_2, RCO_3, HO) \tag{4}$$

Figure 1. Illustration of atmospheric HC and NO_x reaction systems.

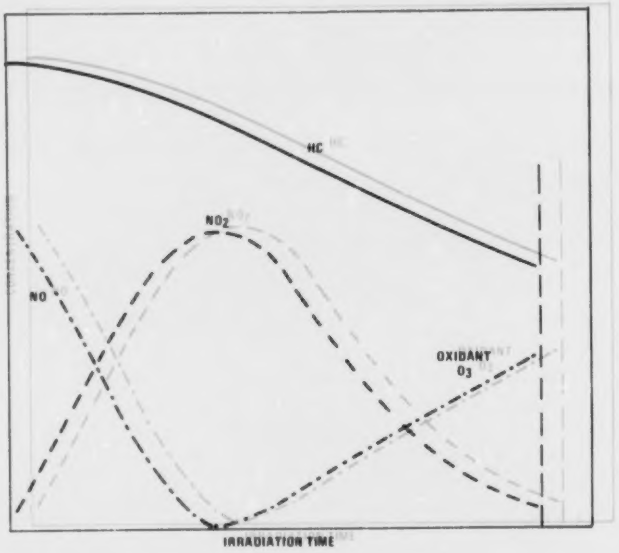


Figure 2. Maximum 1-hour oxidant as a function of NMHC at various NO_x levels.

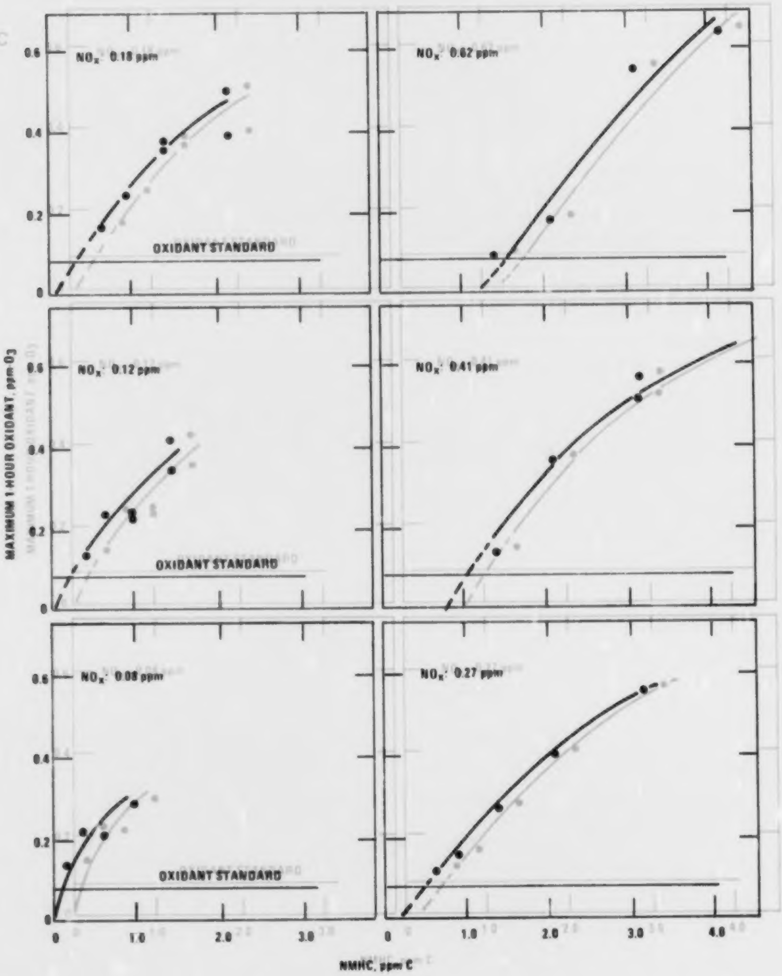


Figure 3. Maximum 1-hour oxidant as a function of NO_x at various NMHC levels ("rational" extrapolation to zero).

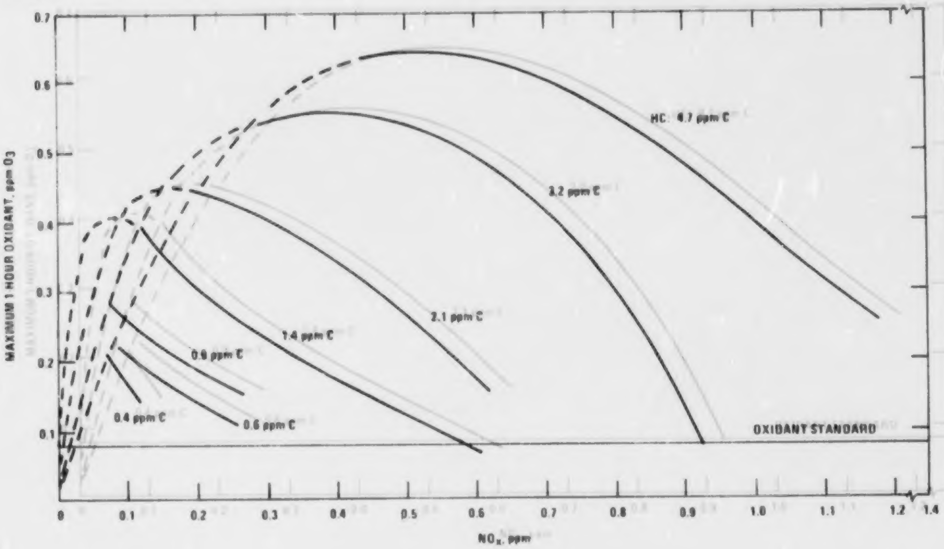
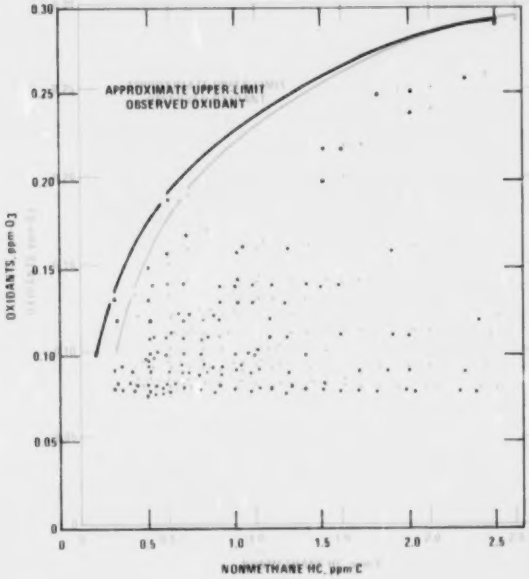


Figure 4. Maximum daily 1-hour-average oxidants as a function of averages of NMHC from 6 to 9 a.m. in several large cities, June through September, 1966 through 1968, and in Los Angeles, May through October 1967.



$$NO + NO_2 + H_2O \rightarrow HONO \xrightarrow{h\nu} HO \qquad (5)$$

$$RO_2 + NO \xrightarrow{O_2} NO_2 + R' \qquad (6)$$

$$R + R' \rightarrow RR' \text{ (e.g., PAN)} \qquad (7)$$

In the absence of HC, O_3 reacts rapidly with NO to regenerate the photolyzed NO_2 so that O_3 accumulation is not permitted. Therefore, in clean air, ambient NO_2 will give little O_3. In the presence of HC, radicals are formed that through chain reactions convert the NO back to NO_2; therefore, O_3 accumulation is now possible. This explains the enhancive effect of HC concentration and HC reactivity.

The NO effect is twofold. First, a relatively simple effect is caused by the fact that O_3 buildup does not start until all NO has been oxidized into NO_2. Therefore, for given irradiation time, higher NO concentration will delay the O_3 formation process and will cause lower O_3 levels. Second, a more complex purely mechanistic effect occurs as follows: The higher the concentration of NO_2 is, the higher the rate of O_3 formation is because there is more NO_2 to photolyze and to form O-atoms and O_3. However, when NO_2 is in large excess (relative to HC), then the $RO_2 + NO \rightarrow NO_2$ step does not remove NO sufficiently fast and NO is left to prevent O_3 from accumulating. This explains the HC/NO effect.

This is an extremely simplified explanation. The process includes perhaps 300 or more reaction steps. However, such detail is not needed for the purposes of this discussion.

PHYSICAL MECHANISM

Physical mechanism is the overall process that starts with the discharge of emissions into the atmosphere above the source areas and terminates with the development of an oxidant problem in the receptor areas. Alternatively, the physical mechanism can be understood as the mechanism that describes the relation between source area and receptor area.

The first mechanism adopted for use was the one that appeared to occur in the Los Angeles basin. By this relatively simple mechanism, referred to here as the local oxidant plume mechanism, the oxidant problem in a locality is caused entirely by the emissions discharged in that same locality. Thus, by this mechanism source area and receptor area coincide. Furthermore, occurrence of such a mechanism means that control of the local emissions is necessary and sufficient for reduction of oxidant in a given locality. This local oxidant plume mechanism is the mechanism adopted by EPA in the development of the oxidant control strategy now in use.

Today it is known that, although this mechanism may be approximated in some localities, it certainly does not have universal validity. Recent studies have revealed that in some localities the oxidant problem is caused by an area oxidant plume, meaning that a significant part of the problem is caused by emissions emitted outside the locality in upwind areas (2). Such an area plume mechanism has been observed to occur in the central and northeast part of the United States; the local plume mechanism appears to be the predominant one in the Los Angeles basin.

METHODS FOR RELATING AMBIENT OXIDANT TO PRECURSOR EMISSIONS

It should be stressed at the outset that all methods now available for relating emissions to oxidant air quality and calculating control requirements are meant to apply to urban air quality only; in fact, they apply only to oxidant formed by the local oxidant plume mechanism. This, of course, is because the oxidant pollution control strategies now in effect are for urban oxidant only.

To relate emission rates to oxidant air quality, we need to quantitate 2 processes: (a) the precursor emission dispersion process and (b) the photochemical reaction process. This has been done—however well or poorly—and the method that resulted is the well-known Appendix J method. This method was derived as follows.

The dispersion process was quantified by assuming a simple rollback model: $C = b + ke$. This led to the well-known simple rollback equation (3):

$$R = \frac{(gf)Cmax - Std}{(gf)Cmax - b} \times 100$$

where Cmax and Std denote present and desired air quality (standard) respectively in terms of pollutant concentration, and gf is the growth factor.

For a primary pollutant, R is the percentage of control of emission needed. For oxidation, however, we need to express Cmax and Std in terms of precursor concentrations because it is the precursor emissions that can be controlled, not the oxidant. Here, the quantification of the photochemical process is needed, that is, a quantitative relation between ambient oxidant concentration and ambient precursor concentration. This relation was obtained from aerometric data in the form of the well-known upper limit curve or envelope curve (Figure 4). This curve was constructed by plotting daily maximum 1-hour oxidant concentration against nonmethane hydrocarbons (NMHC) from 6 to 9 a.m.; both the oxidant and NMHC were measured in the downtown areas of several large cities. From Figure 4 (discussed in the EPA criteria documents for NO_x and HC), one can read off the NMHC values corresponding to Cmax, that is, to the maximum 1-hour oxidant observed in a location, as well as the NMHC value corresponding to Std, that is, to 0.08 ppm O_3. This NMHC value was determined to be 0.24 ppm C, and it is the U.S. air quality standard for HC, which is to be used as a guide only and not as a true air quality standard. By using these NMHC values and the rollback formula, and by assuming $b = 0$ (i.e., no background oxidant or NMHC), the control requirement for the percentage of NMHC was calculated as a function of oxidant concentration, and results (Figure 5) were published by EPA in the form of the Appendix J curve (4).

Appendix J has several limitations arising from the assumptions used in the quantification of both the dispersion process and the photochemical process. But before these limitations are discussed, 4 alternative methods for relating air quality to emissions are presented briefly.

1. Use rollback formula (with $b = 0$) in conjunction with a simple proportionality relation between ambient oxidant concentration and ambient NMHC (or reactive HC) concentration, the latter relation to be used in lieu of the upper limit curve;
2. Use rollback formula in conjunction with oxidant-precursor relations derived from smog chamber data, the latter relations to be used in lieu of the upper limit curve;
3. Use more detailed mathematical expressions for the dispersion process in conjunction with theoretically derived mathematical expressions for the photochemical process (mathematical models); and
4. Use statistically supported empirical relations either between early-in-the-morning precursor levels and oxidant or between emission rates and oxidant within a given area.

Two of these alternative methods, the proportional rollback method and the smog chamber method, are discussed here in more detail.

The proportional rollback method is currently a fairly popular alternative to Appendix J, mainly because it is not based on the highly objectionable upper limit curve and

Figure 5. Required hydrocarbon emission control as a function of photochemical oxidant concentration.

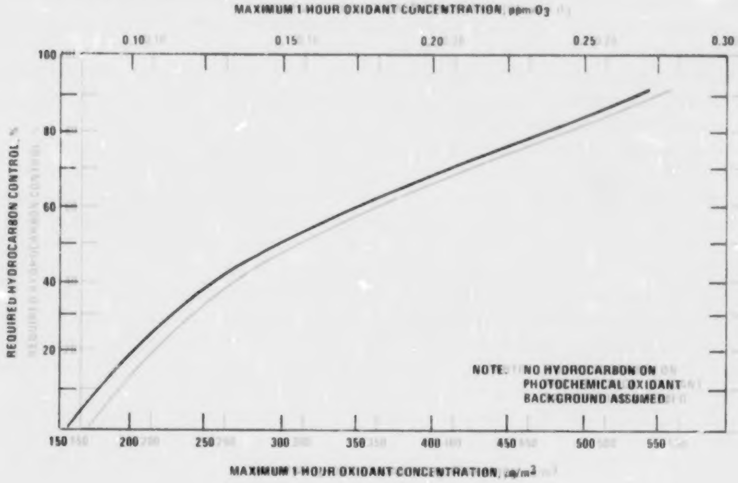
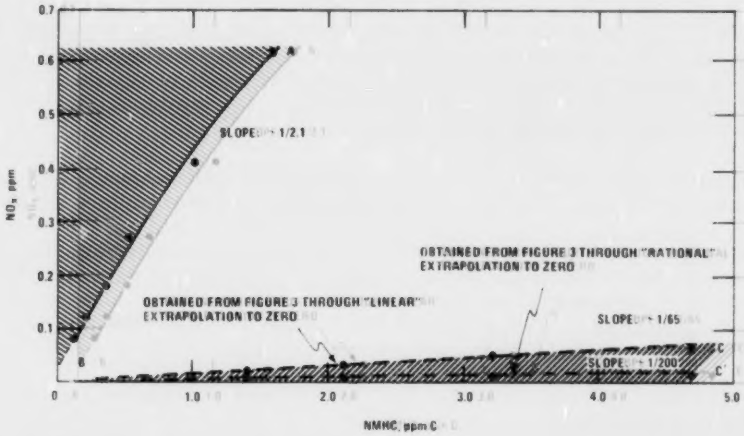


Figure 6. Equal response lines representing combinations of NMHC and NO_x corresponding to oxidant and NO_2 yields equal to the federal air quality standards.



because, relative to Appendix J, it leads to lower control requirements. The key part of the proportional rollback method is the assumption that ambient oxidant is proportional to the reactive hydrocarbon emission rate. The only justification for this assumption is offered by the smog chamber data. Such data show that the oxidant-to-HC dependence is not far from a linear relation (Figure 2). Relative to Appendix J, the proportional rollback method leads to lower control requirements, especially for locations with high oxidant levels.

The smog chamber method is also a popular alternative to Appendix J for the time being, mainly because it considers the role of NO_x quantitatively, a feature that lately has been shown to be an important one, as will be discussed later. The key part of the smog chamber method is the oxidant isopleth diagrams that relate oxidant to both the NMHC and NO_x precursors (Figures 6 and 7). These diagrams were constructed by using data obtained from smog chamber irradiations of HC-NO_x mixtures at varied initial HC and NO_x concentrations. The shaded areas designate the HC-NO_x reactant combinations corresponding to 0.08 ppm O_3 or less. These diagrams reveal one important fact: The higher the ambient NO concentration is, the lower is the requirement for HC control to achieve the oxidant standard. Again, all this pertains only to oxidant formed by the local oxidant plume mechanism.

Specific procedures by which the oxidant isopleths of Figure 8 can be used to calculate numerical control requirements are several, varying in complexity and, presumably, in accuracy also. By the simplest method, it is assumed that the initial reactant concentrations in the smog chamber can be identified with the 6 to 9 a.m. ambient concentrations of HC and NO_x in an urban locality, and the maximum 1-hour O_3 concentration observed in the chamber can be identified with the day's maximum 1-hour O_3 concentration observed in the same urban monitoring site. The accuracy of this method, obviously, depends on how closely the real atmosphere conditions were simulated in the smog chamber. For example, if the chamber light intensity is lower than the sunlight intensity, then the smog chamber data will lead to a degree of control greater than needed. Even if the real atmosphere conditions are closely simulated in the chamber, it is still questionable that the assumption used in this method is valid. This is simply because the reactant (HC, NO_x) and product (O_3) concentrations in the smog chamber obey a cause-effect relation, but the ambient 6 to 9 a.m. HC, NO_x, and later-in-the-day O_3 concentrations do not.

To circumvent the shortcomings of this simple method, LACAPCD investigators (Hamming) offered a technique by which the smog-chamber-predicted O_3 values are mathematically related to the ambient O_3 concentration values (in Los Angeles). This mathematical relation (Hamming transform) is then used to apply smog chamber deductions upon the real atmosphere in Los Angeles. The weaknesses of this LACAPCD method are two: First, the smog chamber data proposed for use are of poor quality; second, the mathematical relation between smog chamber O_3 values and ambient (Los Angeles) O_3 values is unproved. Extensive discussions and critiques of this technique have been presented at technical meetings and published (5, 6). A new method, proposed by this author (7), has the following key steps.

1. The smog chamber data proposed for use are data that have been shown to obey a cause-effect relation reasonably close to the one manifested in a real (urban) atmosphere.
2. The smog chamber counterparts of the ambient HC and NO_x concentrations responsible for observed ambient oxidant are determined from the ambient oxidant value (Cmax, that is, maximum concentration of O_3 observed in reference year) and the ambient 6 to 9 a.m. HC-to-NO_x ratio. Thus, the chamber concentrations of HC and NO_x are obtained from the intersect of the Cmax isopleth and the straight line of the slope equal to the ambient HC-to-NO_x ratio (Figure 7).
3. The so-derived chamber concentration value for NO_x is then reduced as dictated by the NO_2 problem in the locality under consideration.
4. Hydrocarbon control is calculated by taking into consideration that ambient NO_x may vary downward from its maximum value.

Unlike the previous, simpler method, this method does not assume that the 6 to 9 a.m. ambient precursor concentrations are the ones that caused the oxidant concentration observed later in the day; instead, it assumes that the NMHC-to-NO_x ratio in the precursor mixture that caused the observed oxidant has the same value as the ratio in the 6 to 9 a.m. precursor mixture. This latter assumption certainly is a much more valid one, for atmospheric dispersion occurring during the day-long reaction affects the absolute levels of the precursors but not their ratio.

One final point of interest here pertains to the air quality standard for NMHC, that is, the NMHC concentration value corresponding to 0.08 ppm O_3. Based on these chamber data (Figure 7), and considering the unavoidable downward variation of NO_x from

Figure 7. Oxidant isopleths corresponding to various maximum 1-hour oxidant values.

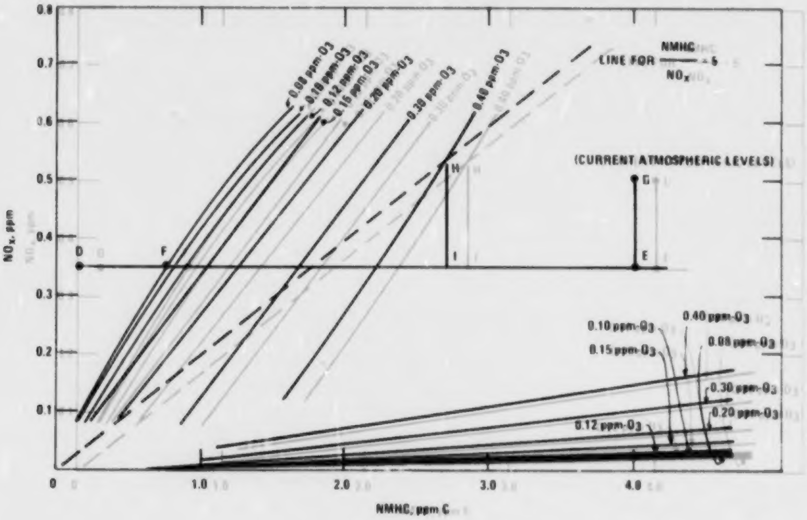
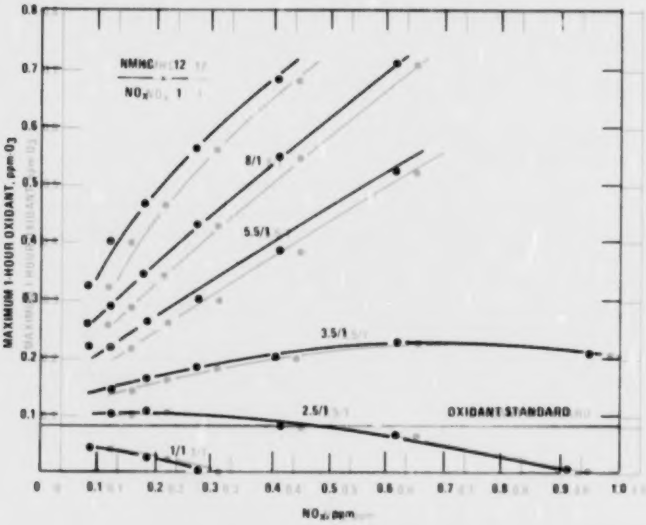


Figure 8. Maximum 1-hour oxidant as a function of NO_x at various NMHC-to-NO_x ratios (smog chamber data).



the maximum NO_x value (dictated by the NO_2 standard), it can be shown that the NMHC concentration corresponding to 0.08 ppm O_3 is about 0.15 ppm C—a value not far off the EPA value of 0.24 ppm C derived from the (upper limit) aerometric data curve (7). Interestingly, using the same smog chamber data, the National Academy of Sciences (NAS) derived an air quality standard for NMHC equal to 0.75 ppm C, that is, 5 times larger in value than the standard derived here (8). However, the NAS derivation ignored the unavoidable daily variation of the NMHC-to-NO_x ratio, an oversight that accounts for the disagreement.

CRITICAL EXAMINATION OF THE METHODS FOR RELATING OXIDANT AIR QUALITY TO EMISSIONS

By far the most important basis for assessing the value of a method is the ability of the method to predict air quality changes from emission changes. Since obtaining pertinent and complete data on emission changes and resultant air quality changes is not possible at present, it follows that direct validation by anyone of the methods available is not possible. This is a problem that is especially serious in the cases of the empirical methods in which the air quality-emission relation does not have a cause-effect nature. It was hoped that this problem could be solved by developing air quality-emission relations based on theory, as in the mathematical modeling methods, and validating such models by using data on absolute (present) air quality. But these hopes have not been justified yet, as will be discussed shortly. For the time being, it appears that the only assessment that can be made of the relative accuracies of the various methods is the one based on qualitative critiques such as the ones presented next.

Critique of the Appendix J Method

The key elements of this method are the upper limit curve depicting the oxidant-to-NMHC dependence, the simple rollback model, and the assumption that there is no background oxidant or NMHC. All 3 elements suffer from inadequacies or uncertainties. The limitations of the upper limit curve are as follows:

1. The curve may depict the dependence of oxidant on the dispersion factor rather than the dependence on the HC reactant factor;
2. The curve depicts a purely empirical relation, not a cause-effect one, and it, therefore, cannot automatically be assumed to have predictive value (it would have a more cause-effect nature if oxidant was measured within the same air mass in which the HC and NO_x measurements were made);
3. The curve disregards the NO_x factor;
4. Experimental error makes the low end of the curve (air quality standard for NMHC) highly uncertain;
5. Scarcity of data points makes the upper part of the curve highly uncertain;
6. The curve is not necessarily valid in locations other than those from which it was derived; and
7. The curve disregards oxidant transport phenomena.

Justification of the upper limit curve relation is mainly based on the following:

1. It is derived from real atmosphere data, a more realistic alternative to smog chamber data;
2. It is in qualitative agreement with the smog chamber data, at least insofar as the oxidant-to-HC dependence is concerned; and
3. It can be improved with the acquisition of additional data.

The simple rollback model also has limitations, the main ones being that it cannot be validated experimentally and that it assumes that all sources behave identically. A more extensive critique has been published (3). The main justification of the model is in its simplicity and in its relatively small demands for input data. The assumption that there is no background oxidant or NMHC is also incorrect, but has been adopted in the interest of simplicity.

Critique of the Smog Chamber Method

The key elements of the smog chamber method are again the rollback model and background oxidant assumption (as in the case of the Appendix J method), and the oxidant-HC-NO_x relations derived from smog chamber data. The limitations of the rollback model and associated assumptions have already been discussed. The limitations of the chamber-derived oxidant-precursor relations are as follows:

1. Chamber atmospheres are only crude simulations of real atmospheres, and chamber data and associated relations, therefore, cannot automatically be assumed to be applicable to real atmospheres; and
2. Chamber data can define oxidant yield as a function of the precursors, but they tell us nothing about the frequency of oxidant occurrence (this inadequacy is significant since the NAQS for oxidant is defined in terms of an oxidant level as well as in terms of a frequency of oxidant occurrence).

Justification of the chamber-derived relations is based on the following:

1. The chamber-derived relations are truly cause-effect relations;
2. The chamber-derived relations are complete in that they involve all controllable oxidant precursors (HC, NO, NO_2);
3. For certain applications, the chamber-derived relations constitute the only option now available, e.g., in development of oxidant control strategies using the approach of coordinated control of HC and NO_x emissions; and
4. Chamber data and associated relations are amenable to improvement.

Critique of the Mathematical Modeling Method

Main input requirements of the mathematical modeling method are emission inventory data, atmospheric reaction mechanism for the emission mixture, and meteorological data. The main limitations of the modeling method arise from the fact that neither the emission inventories nor the reaction mechanism is sufficiently well know, at least now. Another limitation, this one of conceptual nature, arises from the fact that mathematical models cannot be validated directly, i.e., by using real atmosphere data, the main reason being that inhomogeneity makes real atmosphere undefinable, especially at the lower layers. Justification of the mathematical modeling methods is based on the following:

1. They are inherently more valid than the empirical methods, and
2. They are more useful than the other methods.

Discussion of Methods of Relating Emissions to Oxidant Air Quality

All of the existing methods of relating air quality to emissions suffer from uncertainties because of several problems. One problem is that the methods cannot be validated directly since it is not possible to obtain—within a reasonable period of time—pertinent and complete data on emission modification and resultant air quality changes. Validation of a method using data on absolute levels of emissions and air quality (as, e.g., the mathematical model method is to be validated) is also problematic because of the difficulty to uniquely define and quantitate oxidant air quality. Definition and quantitation of such air quality in terms of monitoring data of the usual type are unsatisfactory in that such air quality is not a function of emission rate only; it depends also on the position of the monitoring station relative to the position of emission sources, and on mixing factors—dependencies that are not quantifiable. In the face of this problem, it would perhaps be advisable to abandon the practice of using the customary monitoring data to define and express absolute levels of air quality (such data should be used only to define and express air quality trends). Validation of the various methods would then have to be done somehow else, e.g., against smog chamber data, primarily, and against real atmosphere data secondarily; and predictions by the so validated methods would be used to define and express absolute levels of air quality.

Another problem in the development of useful air quality-emission relations arises from our incomplete understanding of the physical process—by which emissions disperse, react (to form oxidant), and cause oxidant problems in a given area. Most of the existing methods of relating emissions to air quality are based on a simplistic scenario referred to here as the local oxidant plume concept. By this concept, as already discussed, emissions are discharged and dispersed in the air above the source area, react while being continuously diluted and mixed with fresh emissions, and finally cause oxidant pollution that afflicts the very same source area. Recent evidence, however, suggested that the oxidant problem in a locality may be caused by an area oxidant plume. In such localities, it is obvious that certain methods, e.g., the Appendix J method, will have much less validity. Also, monitoring data taken in such localities would be even more inappropriate for validation of mathematical models.

Notwithstanding these imperfections of the existing methods for relating air quality to emissions, a decision has to be made as to which of these methods is the least imperfect one, at the present time, for universal application. Based strictly on technical soundness, my recommendations are as follows.

1. The mathematical model methods are not ready and cannot be used yet—at least not for applications for which other usable methods are available.
2. The statistical emission-versus-oxidant methods are usable only in the localities for which they were developed and validated, and these methods are, therefore, conceptually inappropriate for universal application.
3. The Appendix J, the smog chamber method, and the statistical precursor concentration-versus-oxidant method are the least objectionable ones at present.
4. Of these 3 methods, the Appendix J and the statistical method have the same conceptual and accuracy limitations, already mentioned in the Appendix J critique. The chamber method, therefore, may have a slight advantage over all methods now available. The existing chamber data do not cover the entire range of HC and NO_x combinations of interest. Specifically, data are needed for HC-to-NO_x ratios up to 30:1 and for HC and NO_x concentrations closer to zero. I think that such data could be obtained through the use of a photochemical model developed and validated by using the existing chamber data.

Such an appraisal of the relative merits or drawbacks of the various methods is necessarily a qualitative one. A quantitative comparison, for example, a comparison of the confidence intervals associated with the predictions by the various methods, would be highly desirable, but does not seem to be possible at present or at any time in the future. My recommendations toward an improved method for relating oxidant air quality to emissions are as follows:

1. Conduct field studies, where necessary, to establish the various physical mechanisms by which emissions cause oxidant problems (information from such studies will serve to design appropriate smog chamber studies and to provide the input needed by the mathematical models) and also conduct special field studies to obtain data for validation of mathematical and smog chamber models;
2. Conduct comprehensive smog chamber studies of the O_x-HC-NO_x relations in which properly designed outdoor smog chambers are used and operated under widely diverse static and dynamic conditions, including those that maximize oxidant yield

from given HC-NO_x mixture and those suggested by the field studies on physical mechanism;

3. Use such smog chamber data to develop and validate a mathematical model (use of such diverse data to validate the model might lessen the errors caused by the mechanism uncertainties) and further validate mathematical models with data from special field studies; and
4. Use the validated models to define and express air quality levels in localities or areas and to design control strategies.

ROLE OF NO_x AND OF NATURAL EMISSIONS IN URBAN AND NONURBAN OXIDANT PROBLEMS

The preceding discussion was concerned entirely with the urban oxidant problem. Furthermore, most—but not all—of the methods discussed for relating oxidant to emissions were based on the premise that urban oxidant is an increasing monotonic function of the NMHC reactant; the NO_x role was ignored. Recent findings from field and laboratory studies raised some important implications regarding the relative roles of the NO_x and NMHC reactants, but clearly did not invalidate the premise regarding the NMHC role. Therefore, the control approach now in use—i.e., unilateral control of NMHC—continues to be justified. Some of the specific implications raised by the more recent studies are as follows.

The most important recent finding is the one (from the oxidant transport studies) that led to the distinction between the urban oxidant plume mechanism and the area oxidant plume mechanism by which emissions cause oxidant problems. In areas in which the urban oxidant plume mechanism is the predominant one, the role of NO_x is well understood, thanks to the smog chamber data available. Thus, in such areas emissions should be controlled so as to reduce the HC-to-NO_x ratio in air. In fact, if the ambient HC-to-NO_x ratio is maintained at a low level, e.g., 2.0 or less, it is reasonably certain that the oxidant standard will be achieved (Figure 8). In areas in which the area oxidant plume mechanism is the predominant one, the role of NO_x may be much more complex, as illustrated in the following examples.

1. A suburban or nonurban area has an oxidant problem that is caused almost entirely by man-made emissions transported from upwind areas. The NO_x, in this case, acts as an inhibitor, and control of upwind emissions so as to reduce the HC-to-NO_x ratio will probably be beneficial.
2. A nonurban area has no oxidant problem or has a small problem caused by reactions of local natural HC mixed with man-made (transported or local) NO_x. This is a hypothetical—but not improbable—example of an area in which the natural (local) HC and NO_x emissions alone have an extremely high HC-to-NO_x ratio such that oxidant buildup is not possible or is small. With the injection of additional NO_x, however, such mixtures will develop oxidant producing potential. Therefore, unlike in the previous example, in this example control of upwind NO_x emissions is beneficial. In fact, control of HC alone may be detrimental in that it will cause more NO_x to survive the photochemical process in the upwind areas and to be transported into the nonurban area of this case.

Because of the possibility that the problem in example 2 may be a real one, a sound emission control strategy for oxidant reduction should be designed to ensure that the NO_x levels in air, at least, will not increase as a result of the HC control. Such increase could occur for 2 reasons: first, some methods of controlling HC emission from combustion processes cause an inadvertent increase in NO_x emissions. Second, control of HC to reduce oxidant to 0.08 ppm will cause more NO_x to survive the photochemical process.

In summary, this paper attempts to present a concise picture of the oxidant problem; attention is focused on the aspects thought to be most relevant to the quantitative dependence of ambient oxidant on precursor emissions. Opinions are expressed with the understanding that they should not be taken as representing established or all-accepted viewpoints. Rather they should be taken as a challenge to other viewpoints or a departure point to a review process.

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PHOTOCHEMICAL DIFFUSION MODELS FOR AIR QUALITY SIMULATION: CURRENT STATUS

Kenneth L. Demerjian, Environmental Sciences Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina

The development and implementation of photochemical diffusion models for air quality simulation provide one technique for carrying out the mandates of the 1970 amendments to the Clean Air Act. Mathematical models currently available for evaluating the impact of emissions on air quality consider source emission data, meteorological variables characterizing transport and dispersion processes, and reaction mechanisms describing chemical transformation and removal processes of atmospheric pollutant species. The purpose of this paper is to review and evaluate the status of several photochemical diffusion models currently available. These models, which vary in complexity, were developed to assess the impact of anthropogenic emissions on ambient photochemical oxidant levels in urban areas. Three approaches to photochemical air quality simulation modeling are considered: the grid point model (1, 2, 3, 4), the trajectory model (5), and the box model (6, 7).

PHOTOCHEMICAL AIR QUALITY SIMULATION MODELS

A summary of currently available photochemical air quality simulation models (PAQSM) and their characteristics is given in Table 1 (19). Three of these models were chosen for this evaluation study. A brief discussion of the formulation of the 3 models is given here to provide essential information for the evaluation.

In developing a mathematical relation for simulating the transport, dispersion, and transformation of pollutant emission into the atmosphere, one must consider the following 3 areas.

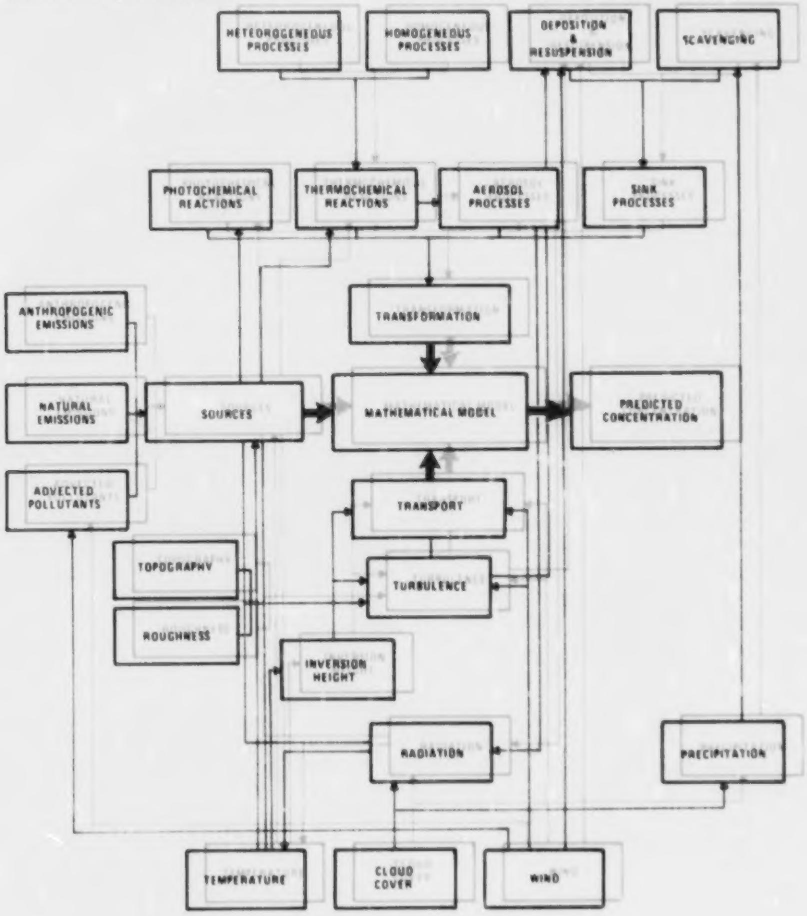
1. Chemical transformation. To understand the relation between $HC\text{-}NO_x$ emissions and photochemical oxidant formation requires that a chemical mechanism be formulated that describes the complex $HC\text{-}NO_x$ oxidation processes occurring in the sunlight irradiated atmosphere.
2. Source emission inventory. Model performance is critically related to the accurate description of the rates of emissions of pollutant species in space and time.
3. Meteorological factor. Methodologies must be developed for the treatment of the meteorological variables that affect pollutant transport and dispersion. The complexity of the methodology used will depend on the mathematical detail considered in describing the transport and dispersion processes in the turbulent planetary boundary layer.

The research and development of each of these areas represent a formidable task. In a latter section of this paper, a discussion and evaluation of the current state of the art of each of these areas are considered. The even greater difficulty of coupling these areas together via mathematical relations describing the physical and chemical dynamics of the atmosphere is the goal of the photochemical air quality simulation model. Figure 1 gives some indication, conceptually, of the complex nature of the

Table 1. Summary of characteristics of photochemical air quality simulation models.

Reference	Description	Results Reported
5	Trajectory model based on moving column of air in which vertical diffusion and chemical reactions take place. Column of air follows surface trajectory interpolated from monitoring station wind readings. Eschenroeder-Martinez kinetic mechanism is used.	Applied to Los Angeles for CO, NO, NO_2, HC, and O_3. Various wind trajectories on 6 validation days. Simulation period per day: 6 to 9 hours.
7	Trajectory model based on well-mixed, moving column of air in which chemical reactions take place. Column of air follows surface trajectory interpolated from monitoring station wind readings. Wayne kinetic mechanism is used.	Applied to Los Angeles for CO, NO, NO_2, HC, and O_3. Various wind trajectories on 6 validation days. Simulation period per day: 4 to 6 hours.
1, 2, 3	Grid model based on numerical solution of 3-dimensional, time-dependent atmospheric diffusion equations. Numerical solution is based on method of fractional steps. Hecht-Seinfeld kinetic mechanism is used. Three-dimensional wind field is computed from surface maps.	Applied to Los Angeles for CO, NO, NO_2, HC, and O_3. Complete spatial and temporal distributions over the basin for 6 validation days. Simulation period per day: 10 hours.
8	Grid model based on numerical solution of 3-dimensional, time-dependent atmospheric diffusion equations. Numerical solution is based on particle-in-cell method. Eschenroeder-Martinez kinetic mechanism is used. Three-dimension wind field is computed from surface maps.	Applied to Los Angeles for CO, NO, NO_2, HC, and O_3. Complete spatial and temporal distributions over the basin for one 16-hour period.
9	Multibox boundary layer model with detailed wind field, vertical profiles of velocity, and diffusivity. Gear's method is used in numerical integration of coupled ordinary differential equations. Lumped chemical kinetic mechanism is used.	Applied to San Francisco Bay Area for CO, NO, NO_2, HC, and O_3. Complete spatial and temporal distributions over the area for several days. Simulation period per day: 24 hours.
6	Cell model based on solution of dynamic mass balance equations with intercell flows neglected, for an array of well-mixed cells. Kinetic mechanism proposed by Friedlander and Seinfeld (14) is used. Single representative wind speed is estimated from available surface measurements.	Applied to Los Angeles for HC, NO, and NO_2. Regional average concentrations predicted for 2 days. Simulation period per day: 6 to 7 hours.

Figure 1. Schematic diagram of major components contributing to photochemical air quality simulation problem.


HETEROGENEOUS PROCESSES
HOMOGENEOUS PROCESSES
DEPOSITION & RESUSPENSION
SCAVENGING
PHOTOCHEMICAL REACTIONS
THERMOCHEMICAL REACTIONS
AEROSOL PROCESSES
SINK PROCESSES
TRANSFORMATION
ANTHROPOGENIC EMISSIONS
NATURAL EMISSIONS
ADVECTED POLLUTANTS
SOURCES
MATHEMATICAL MODEL
PREDICTED CONCENTRATION
TRANSPORT
TOPOGRAPHY
TURBULENCE
ROUGHNESS
INVERSION HEIGHT
RADIATION
PRECIPITATION
TEMPERATURE
CLOUD COVER
WIND

problem to be considered and shows the various interactions occurring among the areas of transport, source emissions, and transformation.

In developing the mathematical relations for describing the physical and chemical dynamics of the atmosphere, it became readily apparent that solutions of the 3-dimensional, time-varying equations for conservation of mass, momentum, and energy for reactive species in the turbulent planetary boundary layer have no practical application in sight. Therefore, simplified approaches had to be adopted for treating the fundamental physical and chemical processes occurring in the atmosphere. Specifically all of the currently available PAQSMs use mathematical relations derived from the observation of mass equation and are based on K-diffusivity theory. Though it is not within the scope of this paper to derive the working equations used by the various PAQSMs (5), it will be useful to write down the working equations and their entailing assumptions for the 3 PAQSMs considered.

The working equation for the grid point model is the most detailed of the 3 model classes considered and is given in equation 1.

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x} K_H \frac{\partial c_i}{\partial x} + \frac{\partial c_i}{\partial y} + \frac{\partial}{\partial z} K_V \frac{\partial c_i}{\partial z} + S_i(x, y, z, t)$$

$$+ R_i(c_1, c_2, \ldots, c_N),\ i = 1, 2, \ldots, N \qquad (1)$$

where

N = number of pollutant species;
c_i = mean concentration of pollutant species i;
x,y,z = Cartesian coordinates;
u,v,w = mean wind speeds in x, y, and z directions respectively;
K_H,K_V = horizontal and vertical turbulent eddy diffusivities respectively;
S_i = rate of injection (or removal) of species i by a volume source (or sink); and
R_i = rate of production (or consumption) of species i through chemical reactions.

In the derivation of equation 1, the following assumptions were made:

1. Pollutant species do not affect atmospheric temperature and velocity, and thus the equations of conservation of species can be solved independently of the equations of momentum and energy;
2. Molecular diffusion is negligible;
3. Atmospheric flow is incompressible;
4. The system is isothermal;
5. Wind velocities and concentrations may be represented as the sum of deterministic and stochastic components;
6. The average value of the stochastic components of concentration is zero;
7. The turbulent fluxes are linearly related to the gradients in the mean concentrations; and
8. Terms of the type $<c_i'c_j'>$ arising from the inclusion of chemical reactions are negligible (c' being the stochastic component of concentration).

In the case of the moving cell or trajectory approach, equation 1 reduces to equation 2

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial z} K_V \frac{\partial c_i}{\partial z} + S_i(x, y, z, t) + R_i(c_1, c_2, \ldots, c_N),\ i = 1, 2, \ldots, N \qquad (2)$$

with the following additional assumptions:

1. The motion of an air parcel corresponds to the local surface wind velocities in the modeling region;
2. Horizontal transport of materials across cell boundaries does not occur; and
3. Variation in wind velocity with height is neglected.

Finally, the box model approach, which assumes constant wind velocity and mixing height and does not consider diffusional effects, reduces to equation 3.

$$\frac{d(c_i)}{dt} = \frac{S_i}{Z} - \frac{uc_i}{\Delta x} - R_i(c_1, c_2, \ldots, c_N),\ i = 1, 2, \ldots, N \qquad (3)$$

where

Z = depth of mixing layer,
Δx = box width, and
u = wind speed.

EVALUATION OF MODELS

The lack of an extensive air monitoring data base needed for carrying out a comprehensive model validation study has necessitated the adoption of alternative approaches to assess model performance. Several techniques will be considered in evaluating the performance of PAQSM. Although, in the final analysis, the evaluations cannot substitute for a validation study, they do provide qualitative and sometimes quantative information on the overall performance of models and their components. In the discussions that follow, evaluations are considered by relating to the basic assumptions made in deriving the working equations, the methodologies and assumptions used by PAQSM components, and the model initial and boundary concentrations.

Evaluating the validity of the diffusion equation has been discussed in detail by Lamb and Seinfeld (11). This work indicates that working equation 1 is a valid representation of atmospheric transport and chemical reactions if the following criteria are met.

1. Source emission function

$$\frac{1}{S_i}\frac{\partial S_i}{\partial t} << 10^{-3}\ \text{sec}^{-1}$$

$$\frac{1}{S_i}\frac{\partial S_i}{\partial x_k} << \frac{1}{2000}\ \text{meter}^{-1},\ k = 1, 2$$

2. Chemical reaction rate

$$\frac{1}{R_i}\frac{\partial R_i}{\partial t} << 10^{-3}\ \text{sec}^{-1}$$

3. Mean velocity components

$$\frac{1}{\bar{u}_i}\frac{\partial \bar{u}_i}{\partial t} << 10^{-3}\ \text{sec}^{-1}$$

$$\frac{1}{\bar{u}_i}\frac{\partial \bar{u}_i}{\partial x_k} \begin{cases} << \frac{1}{2000}\ \text{meter}^{-1},\ k = 1,2 \\ << \frac{1}{20}\ \text{meter}^{-1},\ k = 3 \end{cases}$$

4. Turbulent velocity components

$$\frac{1}{\langle u_i' u_j' \rangle}\frac{\partial \langle u_i' u_j' \rangle}{\partial t} << 10^{-3}\ \text{sec}^{-1}$$

$$\frac{1}{\langle u_i' u_j' \rangle}\frac{\partial \langle u_i' u_j' \rangle}{\partial x_k} \begin{cases} << \frac{1}{2000}\ \text{meter}^{-1},\ k = 1,2 \\ << \frac{1}{20}\ \text{meter}^{-1},\ k = 3 \end{cases}$$

Primed terms in these expressions represent stochastic components of the property, and barred terms represent mean quantities. The limiting conditions, based on measurements of wind turbulence of Lamb and Neiburger (12) and averaging times of 0.3 hour, reflect less stringent limits than expected with hourly averaged data, which is more commonly used. Based on these criteria, model resolution is of the order of 1 hour in time, 8000 m in horizontal space, and 80 m in vertical space. Source emissions and averaging times used by the model should reflect this order of resolution. It should be noted, though, that the above criteria only establish conditions sufficient for the valid application of the diffusion equation. The limiting conditions provide no information with regard to necessity for the valid application of the diffusion equation.

The evaluation of grid and trajectory approaches to PAQSMs has been studied by Liu and Seinfeld (13). Using analytic solutions to simplified forms of the atmospheric diffusion equation, Liu and Seinfeld formulated numerical experiments to assess absolute errors introduced by assumptions made in the 2 modeling approaches. The results of this study are given in Table 2. It should be noted that (a) these results are based on simplified forms of the working equations considered by the PAQSMs and, therefore, may not reflect the true total errors resulting from the assumption; (b) the inclusion of vertical winds in the trajectory approach is quite feasible, but wind shear consideration would seem questionable; and (c) in theory the grid point model can consider wind shear, but currently available models do not include it.

EVALUATION OF METHODOLOGIES AND ENTAILING ASSUMPTIONS USED IN MODELS

As mentioned earlier, the 3 major areas considered in formulating a mathematical model for simulating photochemical air quality are chemical transformations, source emissions, and the meteorological factor. The significant role played by each component in determining the overall performance of a model is considered in this section.

Chemical Transformations

The prediction of photochemical oxidant is critically related to the chemical kinetic mechanism used by the PAQSMs. The development and evaluation of chemical kinetic mechanisms have proceeded by comparing numerical solutions of coupled ordinary differential equations derived from a postulated reaction set, with concentration versus time profiles observed under controlled laboratory conditions for various initial hydrocarbons with NO_x, hydrocarbon-NO_x levels, and hydrocarbon-NO_x ratios. The assumption is that experimental smog chamber studies are analogs of the chemical transformation processes occurring in urban polluted atmospheres. Therefore, chemical kinetic mechanisms that accurately simulate smog chamber results should also accurately simulate chemical reaction processes in polluted atmospheres.

In the early stages of chemical mechanism development for use in the simulation of atmospheric transformation processes, it became readily apparent that inclusion of detailed reaction processes for the individual hydrocarbons present in urban polluted atmospheres was an impossible task. The hundreds of organic species emitted by anthropogenic sources as well as those occurring naturally would necessitate the consideration of thousands of chemical reactions in describing these individual hydrocarbon oxidation processes. Even if all these specific chemical reactions were known and their rate constants determined, their inclusion into the transport model would prove to be a computational nightmare and economically unfeasible. Therefore, techniques had to be devised for generalizing the chemical kinetics such that computational requirements would be met without losing the major features of the hydrocarbon-NO oxidation processes.

The so-called "lumping" technique has become the prevalent approach used by PAQSMs. This technique lumps together the various reactive hydrocarbons present in the polluted atmosphere into one or more classes. Reactions are specified by hydrocarbon class with specific inorganic species (e.g., O-atom, O_3, and HO) that result in the formation of products and lumped hydrocarbon free radical species. The inorganic reactions occurring in the atmosphere are considered specifically, but with varying levels of detail. The following are types of reactions that might be considered in a typical lumped reaction mechanism. A summary of the characteristics of generalized chemical kinetic mechanisms currently in use in PAQSMs is given in Table 3.

$NO_2 + h\nu \rightarrow NO + O$
$O + O_2 + M \rightarrow O_3 + M$
$O_3 + NO \rightarrow NO_2 + O_2$
$O_3 + NO_2 \rightarrow NO_3 + O_2$
$NO_3 + NO_2 \xrightarrow{H_2O} 2\,HONO_2$
$NO + NO_2 \xrightarrow{H_2O} 2\,HONO$
$2\,HONO \rightarrow NO + NO_2 + H_2O$
$HONO + h\nu \rightarrow HO + NO$
$HO + CO \xrightarrow{O_2} HO_2 + CO_2$
$HO_2 + NO_2 \rightarrow HONO + O_2$
$HO_2 + NO \rightarrow HO + NO_2$
$HO + NO_2 + M \rightarrow HONO_2 + M$
$HO_2 + O_3 \rightarrow HO + 2O_2$

$HO + O_3 \rightarrow HO_2 + O_2$
$HC_1 + O \xrightarrow{O_2} a_1 RO_2 + HC_1$
$HC_1 + O_3 \rightarrow b_1 RO_2 + HC_3$
$HC_1 + HO \xrightarrow{O_2} c_1 RO_2 + HC_3$
$HC_2 + HO \rightarrow c_2 RO_2$
$HC_3 + h\nu \xrightarrow{2O_2} RO_2 + HO_2$
$HC_3 + HO \rightarrow RO_2$
$RO_2 + NO \rightarrow RO + NO_2$
$RO + O_2 \rightarrow HC_3 + HO_2$
$RO_2 + NO_2 \rightarrow PAN$
$RO + NO_2 \rightarrow RONO_2$
$RO_2 + O_3 \rightarrow RO + 2O_2$

The sources of errors in the development of generalized chemical kinetic mechanisms stem from 2 primary areas: those associated with the smog chamber data base and those associated with the kinetic mechanism. In the case of chamber data used for mechanism development and verification, errors may be introduced for the following reasons:

1. Inadequate or no control and measurement of levels of H_2O in the chamber,
2. Impurities in background chamber air,
3. Inadequate or no measurements of the spectral distribution and intensity of the chamber irradiation system,
4. Inaccurate or ambiguous analytical methods,

5. Nonhomogeneity due to inadequate stirring or poor chamber design,
6. Adsorption and desorption of reactants and products on chamber walls,
7. Chemical reactions occurring on chamber surfaces, and
8. Inadequate control and measurement of chamber temperature.

Errors associated with the chemical kinetic mechanism include

1. Uncertainties in experimental determinations of specific reaction rate constants;
2. Variations of rate constants with temperature either uncertain or unknown;
3. Inadequacies in lumping due to the nonrepresentativeness of lumped class reactions relative to specific species within the class, e.g., reaction rates, products, and stoichiometric coefficients; and
4. Inaccuracies in the mechanism due to insufficient verification studies.

Smog chamber data available within the past 2 or 3 years have been well characterized with respect to most of the errors outlined above. In these cases, therefore, errors can be taken into consideration in the development and verification of the chemical kinetic mechanism. The major shortcoming in recent years has been the limited quantity of quality smog chamber data available for development and verification of mechanisms.

The sensitivity of the chemical mechanisms to uncertainties in specific reaction rate constants as well as to temperature variations has been assessed by several workers (3, 16, 17). In a recent study by Dodge and Hecht (16), a combined uncertainty and sensitivity factor for reactions was used as an index for ranking possible sources of error in the Hecht, Seinfeld, and Dodge mechanism (15). These results indicated that at least 12 reactions of the generalized mechanism need to be more accurately determined.

Source Emissions

The accurate description of pollutant emissions within some time and space frame is obviously a critical factor in the performance of all types of air quality simulation models. Emissions are usually characterized as being in point, line, or area source configurations. In many cases individual sources may fall into one or more configurations, and the choices made will depend on the particular area and detail emphasized by the model. Table 4 gives some indication of the types of sources considered in each configuration and the necessary input information used by the methodologies. In the development of emissions inventories for PAQSMs, the emphasis is on HC, NO_x, and CO emissions and, therefore, in general, one might consider line sources in more detail than point and area sources. Even this, though, depends on the particular area being modeled.

The overall uncertainties in the generated emission rates can be considerable and will vary with respect to source type, methodology, and quality of input parameters and data used in the emission model. To my knowledge, the only emission models that have undergone some validation are those for point sources. This is not surprising in that line and area source emission validation would be tied directly to the air quality simulation model, which in itself has not yet been validated. Presumably, evaluations of the emission rate estimates can be made based on the overall uncertainties of various components used in the computation. Such an evaluation will not be attempted here, though indications are that uncertainties of the order of ±50 percent in emission rates are not inconceivable.

To gain some insight into the sensitivity of PAQSMs to uncertainties in pollutant emission, Liu and Whitney (18) performed grid point model calculations, varying emission rates uniformly by ±15 percent in individual runs. Comparisons with base calculations showed maximum percentage deviations of the order of 10 percent for CO, 26 percent for NO, 58 percent for O_3, and 17 percent for NO_2. The local maximum deviations were 1.4 ppm for CO, 5.7 pphm for NO, 6.3 pphm for O_3, and 5.7 pphm for NO_2.

Table 2. Evaluation of assumptions used in grid point and trajectory approaches.

Model	Assumption	Errors Introduced
Trajectory	Neglect of horizontal diffusion	<10 percent after 9 hours of simulation
	Neglect of vertical winds	(a) dependent on meteorological conditions and (b) can be as large as 1 order of magnitude
	Neglect of wind shear	(a) dependent on meteorological conditions and (b) can be more than 50 percent after 9 hours of simulation
Grid point	Neglect of numerical errors	(a) dependent on grid cell size, time interval, numerical scheme used, and physical parameters used; and (b) can be as large as 50 percent after 9 hours of simulation

Table 3. Summary of characteristics of generalized chemical kinetic mechanisms.

Reference	Description	Comments
14	Seven-step reaction mechanism that lumps reactive hydrocarbons into single class and assumes O-atom and O_3 as the hydrocarbon oxidizing species. Contains limited information on inorganic reactions.	Limited comparison studies performed with smog chamber data. Does not include HO reactions, which represent major oxidation path for hydrocarbon species. Mechanism has been used in box model approach (5) with limited success.
1, 3	Fifteen-step reaction mechanism that lumps reactive hydrocarbons into single class and assumes O-atom, O_3, and HO as the hydrocarbon oxidizing species. Contains moderate information on inorganic reactions.	Comparison studies performed with 14 smog chamber runs considering 4 hydrocarbon-NO_x systems. HC and NO_x initial conditions used in chamber studies were significantly higher than those observed in urban polluted atmospheres. Mechanism is currently used in grid-point approach (1, 2, 3) with moderate success.
5	Sixteen-step reaction mechanism that lumps reactive hydrocarbons into a single class and assumes O-atom, O_3, and HO as the hydrocarbon oxidizing species. Contains moderate information on inorganic reactions.	Comparison studies performed same as above. Mechanism currently is used in trajectory approach (4) with moderate success.
13	Thirty-nine-step reaction mechanism that lumps reactive hydrocarbons into 4 classes. Hydrocarbon oxidizing species include O-atom, O_3, and HO as well as direct photooxidation for the aldehyde class of hydrocarbon. Contains rather detailed information on inorganic reactions.	Comparison studies performed include above 14 chamber runs and chamber results from an ongoing program at University of California, Riverside. New chamber data base uses HC-NO_x initial conditions more representative of urban polluted atmospheres. Incorporation of mechanism in grid-point approach is under way. Available June 1976.
6	Thirty-three-step reaction mechanisms based on propylene photooxidation. Atmospheric hydrocarbon is specified as propylene and lumped less reactive hydrocarbon species. Hydrocarbon oxidizing species include O-atom, O_3, HO, HO_2, and CH_3O_2.	Comparison studies performed same as in 2 and 3 above. Mechanism currently is used in trajectory approach (6) with moderated success.

Table 4. Emission inventory.

Configuration	Source Type	Methodology Input Parameters
Point	Power plant Large processing plant	Plant identification Spatial coordinates Stack parameters Fuel content Processing materials Operation characteristics Process identification Emission factors Control equipment
Line	Highway, mobile Rail and river vessels	Spatial coordinates Vehicle miles traveled Speed Operation characteristics Vehicle mix Emission factors
Area	Stationary Airports Refineries Off highway, mobile	Spatial coordinates Population distribution Temporal apportioning factors Operation characteristic Emission factors

Note: Emission inventory is distributed in space and time.

Meteorological Factor

All of the PAQSMs developed to date are deterministic in nature; that is, meteorological data are treated entirely as input to the model, and no attempt is made to forecast any meteorological information. Therefore, methodologies must be developed for treating the meteorological data so as to make them amenable to the transport and dispersion portions of the PAQSMs. A summary of the meteorological parameters and related methodologies considered by PAQSMs is given in Table 5. The uncertainties in individual parameters are difficult to assess. Some parameters may be in error by as much as 1 order of magnitude. As with the emissions, an indication of the importance of these parameters on PAQSM predictions can be gained via the sensitivity studies of Liu and Whitney. Table 6 gives their sensitivity analysis results for a grid point PAQSM.

EVALUATION OF INITIAL AND BOUNDARY CONDITIONS OF MODELS

All PAQSMs must take into consideration the initial or boundary or both conditions of the area being modeled. In the case of the grid point approach, boundary pollutant concentrations must be specified for each hour for all grid cells that lie along an inflow boundary from the ground to the inversion base. The horizontal boundary conditions are established, when possible, by using nearby monitoring data as a guide. When such information is unavailable, estimates used are made solely on a judgmental basis. Concentrations are assumed invariant in the Z direction for any given x, y, and t. Initial concentrations are specified in each ground-level grid cell by interpolation using the data collected at monitoring stations during the hour at which the model run is initiated. For trajectory approaches, only initial concentrations need to be specified. The usual approach is to initiate the trajectory in the vicinity of an air monitoring station and use the observed measurements as initial concentrations in the trajectory cell.

To illustrate the importance of boundary concentrations on grid point model calculations, comparative simulations for Los Angeles on September 29, 1969, were made first by using the standard prescribed boundary concentrations and then using a reduced set of nominal boundary concentrations. All other conditions remained the same. Average ozone concentrations for the Los Angeles basin between 1 and 2 p.m. are shown in Figures 2 and 3 for the respective simulations. A comparison of the results shows that only minor differences are observed at the eastern and northern edges of the basin where the maxima occur, but significant differences are observed at the western and central portions of the basin. The overall effect of the reduced boundary conditions was to bring an additional 904 miles^2 (2341 km^2) of the basin below the oxidant standard. This represents a 237 percent improvement in oxidant air quality in the modeling region due to the boundary condition reductions.

The impact of initial conditions on ozone predictions using a trajectory model approach is shown in Figure 4. In this case comparative trajectory simulations were run for Los Angeles on September 29, 1969, for the original initial concentrations prescribed for the cell and ±20 percent of those values.

Even if model performance is assumed quite good, the serious impact that boundary and initial concentrations have on model predictions indicates that these model inputs must be accurately specified. Schemes must be devised for forecasting these input conditions so that impact assessments of various control strategies on future air quality can be made.

VALIDATION OF MODELS

The development and refinement of PAQSMs have proceeded at a reasonable pace during the past several years, but with little or no validation of the models developed. This is due to the lack of an adequate air monitoring data base against which to test the

Table 5. Summary of meteorological parameters and related methodologies considered by PAQSM.

Meteorological Parameter*	Meteorological Data	Related Methodology
Wind field	Wind speed and direction (x, y, z, t)	Linear interpolation Objective analysis Mass consistent approach
Inversion height and thickness	Temperature (x, y, x, t)	Analysis and interpolation of vertical temperature profile when available Data based on climatological observations
Vertical turbulent diffusivity	Turbulent energy dissipation rate, surface roughness, wind speed and direction, and temperature	Lack of sufficient data dictates use of simple empirical relations
Solar radiation	Radiometric (x, y, x, t)	Lack of sufficient data dictates use of functional forms based on clear sky conditions

*All parameters averaged in time and space.

Table 6. Summary of sensitivity of grid point model to variations in meteorological parameters.

Input Parameter	Variation	Local Maximum Deviation	
		CO (ppm)	O_3 (pphm)
Wind direction	Station measurements randomly perturbed by 0 or ±22.5 deg	$\|1.75\|$	
	Values at each grid point randomly perturbed by 0 or ±22.5 deg	$\|2.81\|$	
Wind speed	Station measurements randomly perturbed by 0 or ±1 mph	$\|1.24\|$	
	Values at each grid point randomly perturbed by 0 or ±1 mph	$\|1.73\|$	
	Station measurements decreased by 50 percent	+5.3	+43.7
	Station measurements decreased by 25 percent	+2.4	+24.5
	Station measurements increased by 25 percent	-2.4	-19.6
	Station measurements increased by 50 percent	-4.2	-34.5
Horizontal diffusivity (base value 50 m^2/s)	Decreased to 0	$\|0.04\|$	
	Increased to 500 m^2/s	$\|0.3\|$	
Vertical diffusivity (base value 5 m^2/s)	Decreased to 0.5 m^2/s	+5.8	+36.3
	Increased to 50 m^2/s	-3.0	-16.0
Mixing depths	Decreased by 25 percent	+2.6	+15.3
	Increased by 25 percent	-1.5	-8.5
Radiation intensity	Decreased by 30 percent	0	-19.0
	Increased by 30 percent	0	+14.0

Figure 2. Predicted ozone concentrations in Los Angeles basin using standard model boundary concentrations.

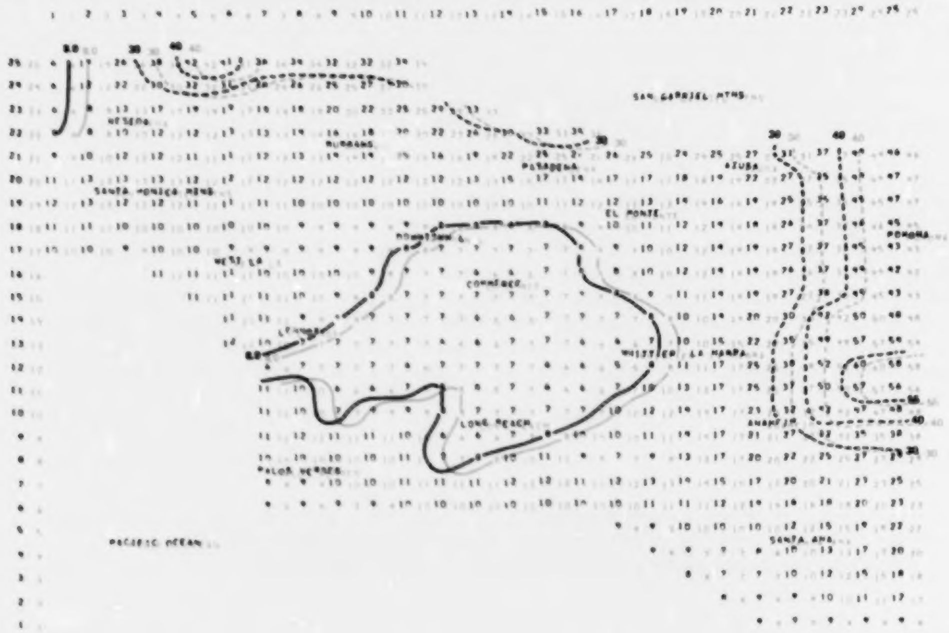


Figure 3. Predicted ozone concentration in Los Angles basin using reduced nominal boundary conditions.

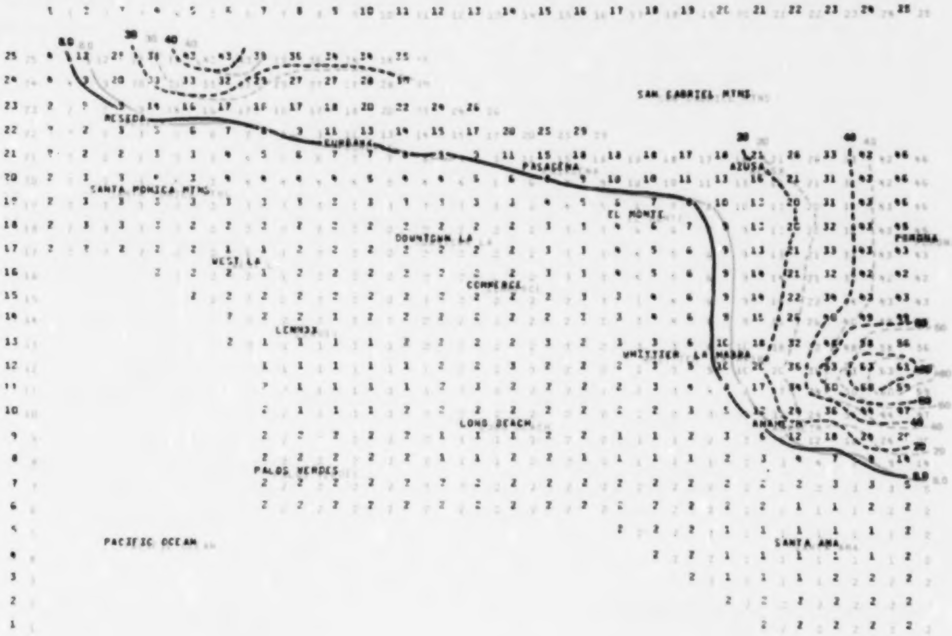
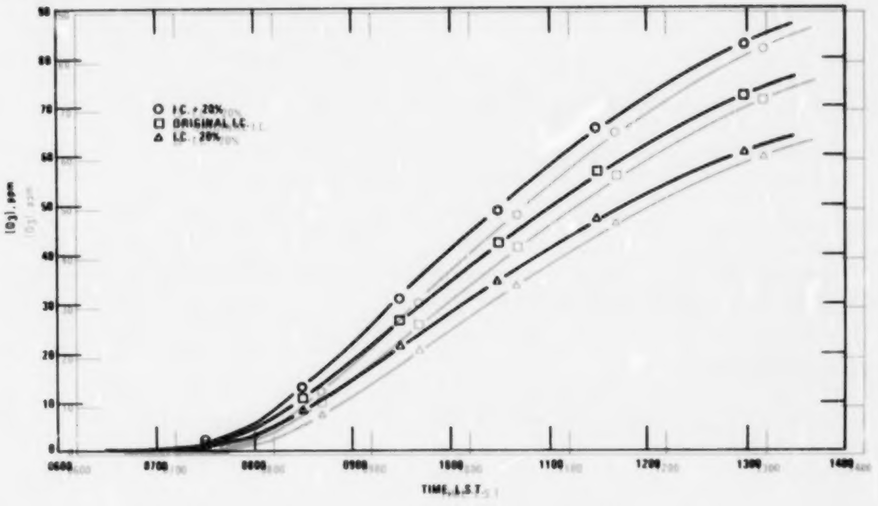

SAN GABRIEL MTNS
RESEDA
BURBANK
PASADENA
AZUSA
SANTA MONICA MTNS
EL MONTE
POMONA
DOWNTOWN LA
WEST LA
COMMERCE
LENNOX
WHITTIER
LA HABRA
LONG BEACH
ANAHEIM
PALOS VERDES
PACIFIC OCEAN
SANTA ANA
8.0
30
40
60

Figure 4. Predicted ozone concentrations in the Los Angeles basin using original and ± 20 percent of initial concentration in trajectory cell.



models. The most extensive testing to date of PAQSMs has been for the 3 models developed under EPA contract (1, 2, 3, 5, 7), which were run on 6 preselected days in the Los Angeles area in the fall of 1969. But even these results must be questioned in that data from many of the monitoring stations used in making comparisons of observed and predicted concentration levels were known to be local source affected and, therefore, did not reflect the spatially averaged concentrations predicted by the models. A statistical analysis of the results from the 3 models previously mentioned has been reported by Liu et al. (18). A tabulation of the statistics has not been presented here, for the results are subject to major interpretation and can be misleading at face value.

Model validation, therefore, provided a major stimulus for the St. Louis Regional Air Pollution Study (RAPS), a 5-year EPA field program initiated in 1972 (20). RAPS objectives include the development and validation of improved air quality simulation models. This requires gathering of an extensive meteorological and air quality data base as well as developing a detailed emission inventory. The monitoring network, which came on line early in 1975, consists of 25 monitoring stations spatially distributed in a spiral configuration covering approximately a 2500-mile^2 (6400-km^2) area. The measurements include total and nonmethane HC, total sulfur, H_2S, SO_2, NO, NO_2, NO_x, CO, total suspended and fine particulate, wind speed and direction, temperature, dew point, barometric pressure, back scatter, and solar radiation.

The model validation studies, encompassing scores of comparisons between computer simulations and monitoring data, will provide the first adequate set of statistical criteria on which to judge model performance. This will, in the final analysis, provide the necessary information for assessing and selecting models for various application purposes.

SUMMARY AND CONCLUSIONS

This paper provides an overview of the various photochemical air quality simulation models currently available and considers evaluations for the various assumptions, methodologies, and input used by the model. The results indicate that the potential for serious error is present in every PAQSM currently available and that extensive verification is necessary to assess the accuracy and utility of these models.

It should be noted, though, that, even in their present uncertain form, PAQSMs provide unique information unavailable from currently applied methods for relating ambient oxidant to precursor emissions. One such example is the ability of PAQSMs to resolve, both in space and time, the impact of new precursor source emissions on ambient levels of oxidant. Therefore, some exercising of the models may be warranted to provide insight into problems for which no other techniques are currently available. This would especially be reasonable in areas where the models have been used or where data bases sufficient to run the models exist.

Verification studies for PAQSMs under RAPS are scheduled to begin in the fall of 1976. Preliminary assessment of several models should be available by early 1977. With the completion of verification and sensitivity studies, an evaluation will be made regarding potential applications of the models.

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ACCURACY OF PREDICTION OF URBAN AIR POLLUTANT CONCENTRATIONS BY DIFFUSION MODELS

John H. Seinfeld, California Institute of Technology

Projections of future transportation-related air quality impacts require the use of mathematical models that relate emissions to air quality. Whereas the derivation and use of such models have received much attention (at least for inert pollutants, such as CO), much less attention has been paid to questions of the interpretation of the concentrations these models predict and how the predictions relate to real atmospheric quantities. Concepts of validity and accuracy must be carefully defined for any model that is to be used in order that the predictions from the model can be properly evaluated. The purpose of this paper is to formulate the concepts of validity and accuracy for atmospheric air pollutant diffusion models and to suggest numerical experiments that can be used to test both the validity and the accuracy of the models.

VALIDITY OF ATMOSPHERIC DIFFUSION EQUATION

All conventional atmospheric diffusion models are based on the equation of conservation of mass:

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = D_i\left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2}\right) + R_i(c_1, \ldots c_N, T) + S_i(x,y,z,t) \qquad (1)$$

where c_i is the concentration of species i; u, v, and w are the fluid velocities in the 3 coordinate directions; D_i is the molecular diffusivity of species i in air; R_i is the rate of generation (or the negative of the rate of disappearance) of species i by chemical reactions at temperature T; and S_i is the rate of injection of species i into the fluid from sources.

Because the atmosphere is a turbulent flow, the velocities u, v, and w are random functions of space and time. Consequently, the concentration c_i is also a random function of space and time. Solutions of equation 1 with realistic atmospheric velocities are difficult to obtain, even in the case in which $R_i = 0$ (inert species). To render equation 1 solvable, the fluid velocities are decomposed into mean and fluctuating components, $u = \bar{u} + u'$ and so on. The quantities $\bar{u}$, $\bar{v}$, and $\bar{w}$ represent the ensemble mean velocities of an infinite number of realizations of the same flow. Correspondingly, we can divide c_i into $\bar{c}_i + c_i'$, where $\bar{c}_i$ is the ensemble mean concentration (23).

Substituting the mean and fluctuating terms into equation 1 and averaging the resulting equation over the ensemble of flows, we obtain the equation governing $\bar{c}_i$. In atmospheric applications, the molecular diffusion term is negligible when compared to that representing advective transport. Thus, neglecting the contribution of molecular diffusion, the equation for $\bar{c}_i$ is

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}\frac{\partial \bar{c}_i}{\partial x} + \bar{v}\frac{\partial \bar{c}_i}{\partial y} + \bar{w}\frac{\partial \bar{c}_i}{\partial z} + \frac{\partial}{\partial x}\overline{u'c_i'} + \frac{\partial}{\partial y}\overline{v'c_i'} + \frac{\partial}{\partial z}\overline{w'c_i'} = \overline{R_i(c_1, \ldots, C_N, T)}$$

$$+ \bar{S}_i(x,y,z,t) \qquad (2)$$

We note the emergence of the new variables $\overline{u'c_i'}$, $\overline{v'c_i'}$, $\overline{w'c_i'}$, which represent the fluxes of species i in the 3 coordinate directions as a result of the velocity fluctuations, u', v', and w'. If species i is involved in second-order chemical reactions, then the term $\bar{R}_i$ will also lead to new dependent variables of the form $\overline{c_i'c_j'}$. For example, if species i decays by a second order reaction $I + I \xrightarrow{k}$, then the mean rate of disappearance of species i is given by $\bar{R}_i = -k\overline{c_i^2} = -k\bar{c}_i^2 - k\overline{c_i'^2}$, where the first term is the contribution to the mean rate of reaction from the mean concentration and the second term is the contribution to the mean rate of reaction from the fluctuating concentration. We see that in this case the new dependent variable $\overline{c_i'^2}$ enters equation 2.

Equation 2 is a rigorously valid equation for $\bar{c}_i$ (neglecting, of course, molecular diffusion): and, if the variables $\overline{u'c_i'}$, $\overline{v'c_i'}$, $\overline{w'c_i'}$, and any of those arising from $\bar{R}_i$ are known as functions of space and time, it can be solved in principle to yield $\bar{c}_i$. Unfortunately, $\overline{u'c_i'}$ and so on cannot be measured at all points in an atmospheric flow and cannot be predicted exactly because of the closure problem of turbulent flow. Thus, we must resort to models for these terms. The model employed in virtually all cases in which atmospheric flows are involved is that based on the concept of eddy diffusivities:

$$\overline{u'c_i'} = -K_H\frac{\partial \bar{c}_i}{\partial x} \qquad \overline{v'c_i'} = -K_H\frac{\partial \bar{c}_i}{\partial y} \qquad \overline{w'c_i'} = -K_V\frac{\partial \bar{c}_i}{\partial z} \qquad (3)$$

The eddy diffusivities K_H and K_V are postulated to be functions of space and time (and not of $\bar{c}_i$ or any of its gradients).

Although there has been some study of the nature of terms of the form $\overline{c_i'^2}$ arising from turbulent chemical reactions, no atmospheric diffusion models for chemically reactive pollutants currently include expressions for these terms. All models employ the approximation

$$\overline{R_i(c_1, \ldots, c_N, T)} \simeq R_i(\bar{c}_1, \ldots, \bar{c}_N, T) \qquad (4)$$

The result of using equations 3 and 4 in equation 2 is the so-called atmospheric diffusion equation (ADE):

$$\frac{\partial \bar{c}_i}{\partial t} + \bar{u}\frac{\partial \bar{c}_i}{\partial x} + \bar{v}\frac{\partial \bar{c}_i}{\partial y} + \bar{w}\frac{\partial \bar{c}_i}{\partial z} = \frac{\partial}{\partial x}\left(K_H\frac{\partial \bar{c}_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H\frac{\partial \bar{c}_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V\frac{\partial \bar{c}_i}{\partial z}\right)$$

$$+ R_i(\bar{c}_1, \ldots, \bar{c}_N, T) + \bar{S}_i(x,y,z,t) \qquad (5)$$

Equation 5 is the fundamental equation on which most current urban air pollution models for photochemical pollutants are based.

The validity of the atmospheric diffusion equation relates to how closely the predicted mean concentration $\bar{c}_i$ corresponds to the true ensemble mean concentration. If the mean velocities, $\bar{u}$, $\bar{v}$, and $\bar{w}$, are known precisely at all points as a function of time, then for an inert species, the only source of a discrepancy between the predicted and true mean concentrations is the eddy diffusivity model for the turbulent fluxes. Thus, for an inert species, the only source of invalidity of the atmospheric diffusion equation is, in principle, the eddy diffusivity closure of the turbulent flux terms.

If the true ensemble mean velocities and concentrations are known for an atmospheric flow, then it is relatively straightforward to assess the validity of equation 5 for specified forms of K_H and K_V. Unfortunately, for any atmospheric flow the ensemble mean velocities and concentrations can never be computed since the atmosphere presents only one realization of the flow at any time. (Of course, for a statistically stationary flow, ensemble averages can be replaced by time averages. The atmosphere is, however, seldom in a stationary condition for any appreciable period of time.) Figure 1 shows a hypothetical relation among the instantaneous concentration measured at a point, the ensemble mean concentration at that point (which is unknown), and the mean concentration predicted by the atmospheric diffusion equation at the same point. Because the true mean velocities that are required to solve equation 5 and the true mean concentration with which the solution of 5 is to be compared are not available in general, an unambiguous measure of the validity of equation 5 for any particular flow cannot be obtained.

To assess the validity of equation 5 requires a flow field for which all desired statistics can be obtained. Since the measurement requirements needed to obtain such statistics in the atmosphere are so overwhelming as to be totally impractical, one must turn to numerical simulations of turbulent flow to provide a flow field within which to perform atmospheric diffusion "experiments." (Such numerical simulations are not, of course, completely exact representations of turbulent flow since a closure assumption must be invoked at some point in the solution of the equations. In Deardorff's simulation the sub-grid-scale turbulent transport becomes a parameter by an eddy viscosity.) Apparently the only examination of the validity of conventional atmospheric diffusion theories with such a numerical simulation is that of Lamb et al. (17), in which a continuous line source was embedded in Deardorff's planetary boundary layer model (4). The mean concentration of an inert pollutant issuing from the line source was computed by averaging over individual particles released in the nearly stationary and homogeneous flow. The "real" mean concentration was then compared to that predicted by the atmospheric diffusion equation as well as conventional Gaussian puff and plume formulas. With the availability of the planetary boundary layer simulation of Deardorff, a number of numerical experiments are possible to assess the validity of the atmospheric diffusion equation.

1. Theoretical forms for eddy diffusivities, particularly K_V, can be tested by comparing the mean concentration field predicted by the diffusion equation with the "true" mean concentration field. [Experiments of this type were carried out by Lamb et al. (17), and further work by Lamb is still in progress.]
2. Chemically reacting flows can be simulated by direct solution of equation 1. True mean concentrations can be determined by time-averaging the resulting concentrations (since the flow is essentially stationary). Then closure approximations for terms of the form $\overline{c_i'c_j'}$ can be evaluated by comparing the solution of the atmospheric diffusion equation to the data. (Work is in progress on this aspect by Wengle and Seinfeld.)

In summary, assessment of the validity of the atmospheric diffusion equation is an extremely difficult task owing to the fact that mean concentrations for actual flows are nearly impossible to obtain. However, with the advent of numerical turbulence simulations, such as that of Deardorff, such assessments are becoming feasible and will be important areas for future investigation.

ACCURACY OF ATMOSPHERIC DIFFUSION EQUATION

Whereas validity refers to the extent of agreement of the mean concentrations predicted by the atmospheric diffusion equation with those from an actual flow, accuracy refers to the extent of agreement between the mean concentrations predicted by the model based on the diffusion equation and those predicted by the equation with the true values of all input parameters. Thus, if $\bar{u}$, $\bar{v}$, and $\bar{w}$ are the true mean velocities, $\bar{R}_i$ is the true chemical reaction rate, and $\bar{S}_i$ is the true source emission function, a $\bar{c}_i$ will be predicted that can be taken as the most accurate concentration achievable with that equation. Errors introduced as a result of the facts that $\bar{u}$, $\bar{v}$, and $\bar{w}$ are not the actual mean velocities, $\bar{R}_i$ may not be based on the actual reaction mechanism, and $\bar{S}_i$ is not the true source emission function will serve to reduce the accuracy of the model when compared to the most accurate achievable.

Table 1 gives the errors inherent in most urban diffusion models; errors are classified according to whether they are a source of invalidity or inaccuracy. Table 2 gives the sources of discrepancy between the mean concentration predicted by the atmospheric diffusion equation and the concentration measured at a particular location in an urban area. The sources of errors in the atmospheric diffusion equation are shown in Figure 2.

The inputs needed to solve ADE together with possible sources of error in those inputs are given in Table 3. In this section we discuss each input and the likely level of error associated with that input. In each instance unless the actual value of the input is known, the level of error in that input can only be estimated. From the standpoint of the effect of errors on the predictions of the equation, joint consideration must be given to the level of uncertainty in each input parameter and the sensitivity of the predicted concentrations to the parameter. Uncertainty relates to the possible error in the parameter from its true value, and sensitivity refers to the effect that variation in that parameter has on the solution of the equation. A parameter may have a large uncertainty associated with it but have little influence on the solution. In such a case, effort at reducing the uncertainty in the parameter value may be unwarranted. On the other hand, small uncertainties in a parameter to which the solution is quite sensitive will have a large impact on uncertainties in the predicted concentrations. Thus, both uncertainty and sensitivity must be considered when the accuracy of the atmospheric diffusion equation is evaluated.

Meteorological Inputs

Practical difficulties of solving the coupled mass, momentum, energy, and species continuity equations for atmospheric pollutant dynamics create a situation in which only the continuity equations of the form of equation 5 are used. The implication of using only the species continuity equation is that a description of the wind field at a resolution equivalent to the grid is required. Unfortunately, the atmospheric measurements required to specify the state of the wind field to this level of accuracy are usually not available. Because the wind field can be specified in terms of only a limited number of observations on a much coarser grid than that on which equation 5 is solved, individual fluid motions with scales smaller than the grid are uncharacterized. A key problem in the use of equation 5 is how to create from the observed meteorology information that is required for the solution of equation 5.

There are 2 basic approaches to obtaining the wind field; the objectives in both cases are to represent the wind field in a way that minimizes irregularities and observational errors. Traditionally meteorologists have drawn isopleths and then used them as a basis for estimating the wind components. An obvious problem with this method is that any one analysis is subject to personal interpretation. The problems of this subjective technique can be avoided if the meteorological variables are objectively related to the space coordinates.

Objective analysis techniques are now used on a routine basis to construct fields of optimized meteorological variables at specified model grid points from irregularly

Figure 1. Hypothetical relations among concentrations.

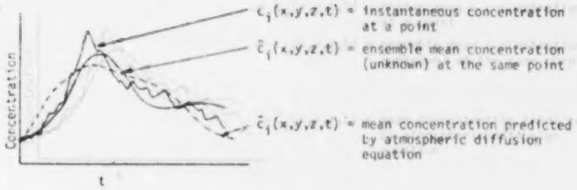

Table 1. Errors in the atmospheric diffusion equation.

Source of Error	Type of Source and Error	Comment
True form of the turbulent fluxes, $\overline{u'c'_i}$, $\overline{v'c'_i}$, and $\overline{w'_i}$, is unknown	Major source of invalidity of atmospheric diffusion equation (ADE)	Higher order closure models will offer improvement over eddy diffusivities in representing these terms
Chemical reaction mechanism R_i does not accurately reflect the actual chemistry	Source of invalidity for chemically reacting species	Continued study of laboratory chemistry and its relation to atmosphere needed to minimize this source of error
Turbulent fluctuating chemical reaction terms are neglected	Secondary source of invalidity of ADE	Closure models appropriate for turbulent chemistry can be developed
Mean velocities $\overline{u}$, $\overline{v}$, and $\overline{w}$ used in solution of ADE are not true ensemble means (usually $\overline{u}$, $\overline{v}$, and $\overline{w}$ are constructed from data at a finite number of locations)	Source of inaccuracy of ADE	There is no way to determine true mean from data; $\overline{u}$, $\overline{v}$, and $\overline{w}$ can be calculated from accurate fluid mechanical turbulence model
Source emission function S_i is inaccurate	Source of inaccuracy	Better compilation of emission factors needed
ADE must be solved on a grid of a size consistent with spatial detail in wind and source emission functions	Source of inaccuracy	Better resolution of wind and source emission fields will allow use of finer grid

Table 2. Discrepancies between predicted and measured concentration.

Source of Discrepancy	Possible Remedy
Concentration measured on a given day is result of random event	None
Concentration is measured at a point, but ADE is applied to a grid volume	Reduce grid size in calculation Place monitoring point at a location where air quality is representative of a region the order of the grid size Develop a sub-grid-scale model
Measurement errors	Better monitoring equipment

Figure 2. Sources of errors in atmospheric diffusion equation.

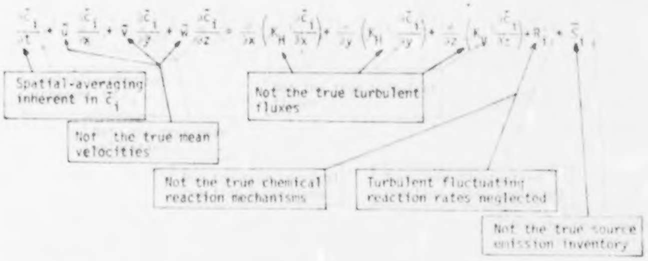
Spatial-averaging inherent in $\tilde{c}_i$
Not the true mean velocities
Not the true turbulent fluxes
Not the true chemical reaction mechanisms
Turbulent fluctuating reaction rates neglected
Not the true source emission inventory

Table 3. Inputs needed to solve atmospheric diffusion equation.

Input	Level of Detail	Sources of Error
Wind velocities	Variation of $\overline{u}$, $\overline{v}$, and $\overline{w}$ with x, y, z, and t	Measurements available only at a few locations, generally at ground level, at discrete times Erros in variation of $\overline{u}$ and $\overline{v}$ horizontally, variation of $\overline{u}$ and $\overline{v}$ vertically, and determination of $\overline{w}$
Eddy diffusivities	Variation of K_H and K_V with z and t	No direct measurements available K_H and K_V must be inferred from theories Both magnitude and vertical variation unknown
Chemical reaction mechanism	Rate equation for each $\overline{c}_i$	Inaccurate rates because of inability to simulate atmosphere in laboratory, unknown reactions, and unknown rate constants
Source emissions	Emission rate as a function of x, y, z, and t	Inaccurate knowledge of level of source activity and emission factors
Boundary conditions	Location of vertical boundary as a function of x, y, and t	Lack of data or adequate model of temperature structure of atmosphere

spaced observational data. Panofsky (25) introduced objective analysis with a technique of using cubic polynomials to fit observed pressure data and obtaining the coefficients from a least squares analysis. Independent polynomials were obtained for separate areas with the consequence that, at the boundaries, the field was discontinuous. Since the discontinuity has no physical basis, a method that smooths the data along the edges is necessary. Gilchrist and Cressman (14) modified the approach of Panofsky by considering only the data surrounding the grid point and then fitting a "most probable" second order polynomial to the observation. This procedure conforms to conventional synoptic practice in that it does not include data in remote parts of the region as implied by any method using Fourier analysis or polynomial fitting to the whole region.

Some improvements can be made on the interpolation and matching stages (13). One example to create an initial approximation of the field at a point (x,y) is to use polynomial surface fitting with the data for the least squares analysis weighted by an equation of the following type:

$$\bar{u}(x,y,0,t) = \sum_{i=1}^{M} f(x - x_i,\ y - y_i)\, u^{obs}(x_i,y_i,t) \tag{6}$$

Liu and Goodin (19) and Liu and Perrine (20) omitted the surface fitting and simply used a least squares form of f with the number of data points, M, dictated by observations within a specified radius around (x,y). There are various other schemes, the simplest being to use the value of the nearest observation. Wind fields created by these techniques are not, however, necessarily consistent with the condition of mass conservation.

Interpolation and surface-fitting techniques can be used as an initial basis for subsequent operations that remove the artificial divergence and convergence introduced by numerical and observational errors. The most common approaches have been to apply various iterative schemes to minimize the divergence of 2-dimensional wind fields in an attempt to satisfy the constraint:

$$\frac{\partial h}{\partial t} + \frac{\partial (uh)}{\partial x} + \frac{\partial (uh)}{\partial y} = 0 \tag{7}$$

where h is the height of the inversion base above the topography and u and v are the x and y components of $\underline{u}(x,y,0,t)$. When the approximation schemes are used, a residual other than zero appears on the right side of equation 7, i.e.,

$$\frac{\partial h}{\partial t} + \frac{\partial (uh)_a}{\partial x} + \frac{\partial (uh)_a}{\partial y} = \epsilon \tag{8}$$

where $( )_a$ indicates that the approximate values are used. Sasaki (28) introduced a method based on variational calculus that allows for the adjusted values of the dependent variables to satisfy exactly an imposed constraint ($\epsilon = 0$). Sasaki demonstrated that a Lagrange multiplier λ should satisfy

$$\nabla^2 \lambda = -\frac{\partial h}{\partial t} + \frac{\partial (uh)_a}{\partial x} + \frac{\partial (uh)_a}{\partial y} \tag{9}$$

with $\lambda = 0$ on the domain boundaries. The adjusted values of u and v can be determined from a solution of equation 9 by using

$$uh = (uh)_* + \frac{\partial \lambda}{\partial x} \qquad vh = (uh)_* + \frac{\partial \lambda}{\partial y} \tag{10}$$

Sasaki (30, 31, 32) introduced a modification of his original formulation by allowing for a reduction of ϵ over the grid not necessarily forcing $\epsilon = 0$ during adjustment. Dickerson (6, 7) used both formulations to develop mass consistent wind fields for the San Francisco Bay Area (18). Endlich (9, 10) and Endlich and Mancuso (11) developed a point iterative scheme that minimizes the divergence but at the same preserves the vorticity. Liu and Goodin (19) have compared these techniques and their practical validity in creating wind fields for the Los Angeles basin. As a result of their work on the Sasaki and Endlich methods, they proposed a model using the best features of both techniques. The usual method of computing nondivergent and irrotational wind fields is to solve Poisson equations for the stream function and velocity potential (1, 2). There are important practical difficulties with this approach because of the difficulty of specifying satisfactory boundary conditions (15).

Of the approaches described above, most have been applied to the generation of 2-dimensional fields. Lange (18) employed Dickerson's technique to specify a 3-dimensional wind field for a particle in cell formulation of equation 5 for conservative pollutants. Until quite recently most 3-dimensional models of pollutant transport have used subjectively prepared wind fields. Meteorological inputs to the current version of the model of Systems Applications, Inc., have been prepared from observational data by using the methods of Fankhauser (12) and O'Brien (24).

Fankhauser used the horizontal wind field u(x,y,t) to obtain a vertical profile of divergence at each grid point using

$$D_K = \frac{\partial u}{\partial x} + \frac{\partial N}{\partial y} \tag{11}$$

where the horizontal velocity components are the mean for each grid cell of thickness K. With the use of the continuity equation, integration of the divergence profile with respect to pressure gives the vertical component of velocity w_p at the top,

$$w_p = w_{p+\Delta p} + D_K \Delta p \tag{12}$$

The vertical velocity computed in this way generally produces reasonable values at low levels, but leads to physically unrealistic results in the upper layers. This is a problem common to many techniques and is primarily attributable to the fact that the quality of wind measurements (as distinct from pressure) deteriorates with increasing elevation angles because of the combination of winds aloft and short sounding duration.

O'Brien (24) developed a scheme used by Fankhauser for altering the original divergence estimates so that the adjusted profiles satisfy some independently defined boundary condition on w at the inversion base and at ground level. The method is based on the hypothesis that divergence errors increase vertically as a linear function of pressure.

The generation of mass consistent wind fields can be achieved by a number of techniques. Which method produces the best result is largely a question of the quality of the observational data and the degree to which the field is constrained by boundary conditions. Incorporation of the effects of wind shear and different vertical velocity profiles should really be considered only if there are sufficient observational data to determine the power law exponents. (The RAPS study in St. Louis should provide experimental data on wind fields aloft to resolve some of the presently unknown boundary conditions.) Until complete planetary boundary layer models can be developed and validated, photochemical modeling must continue to rely on the use of mass consistent wind fields derived from observational data.

Chemical Reaction Mechanisms

Because of the large number of hydrocarbon species in urban air, generalized kinetic mechanisms capable of inclusion in the diffusion equation had to be developed. The source of errors in generalized kinetic mechanisms for photochemical smog are twofold (5):

1. Errors in simulating atmospheric reactions in the laboratory—(a) inadequate or no control and measurement of levels of H_2O in the chamber, (b) impurities in background chamber air, (c) inadequate or no measurement of the spectral distribution and intensity of the chamber irradiation system, (d) inaccurate or ambiguous analytical methods, (e) nonhomogeneity due to inadequate stirring or poor chamber design, (f) adsorption and desorption of reactants and products on chamber walls, (g) chemical reactions occurring on chamber surfaces, and (h) inadequate control and measurement of chamber temperature; and
2. Errors associated with the chemical kinetic mechanism—(a) uncertainties in experimental determinations of specific reaction rate constants, (b) variations of rate constants with temperature either uncertain or unknown, (c) inadequacies in lumping due to the nonrepresentativeness of lumped class reactions relative to species within the class, e.g., reaction rates, products, and stoichiometric coefficients, and (d) inaccuracies in the mechanism due to insufficient verification studies.

As Demerjian points out, most recent smog chamber data have been well characterized with respect to the first category above. A combined uncertainty and sensitivity study of the Hecht, Seinfeld, and Dodge (16) kinetic mechanism for photochemical smog has been carried out by Dodge and Hecht (8). In that study it was found that several reactions previously included in the mechanism have little effect on the concentration predictions and can be neglected. It was also found that the rate constants of 12 reactions should be more accurately determined. It is important to note that this study was concerned not with the validity of the mechanism vis-à-vis atmospheric chemistry, only with the uncertainty of the rate constants and the sensitivity of the concentrations to those rate constants. Thus, assuming that the mechanism is a valid representation of atmospheric chemistry, the study will determine the level of uncertainty in predicted concentrations resulting from uncertainties in rate constants. Although the Dodge and Hecht study was carried out for a batch laboratory system, the combined uncertainty-sensitivity results will apply in atmospheric calculations.

Source Emissions

Source emissions from each class of source can be characterized according to

1. Level of spatial resolution,
2. Level of temporal resolution, and
3. Uncertainty in emission quantity, i.e., in source activity or in emission factor.

The level of spatial resolution achievable is generally as fine as one desires since the locations of all sources can presumably be specified (although traffic count data may not be available on a street-by-street basis). Temporal emission rates will fluctuate some from day to day. For motor vehicles it is safe to use single temporal distributions for surface streets and freeways derived from the analysis of appropriate data. Emissions from some stationary sources may vary with ambient temperature, but these variations are generally known as a function of temperature. The major problem in properly specifying source emissions is uncertainty in emission quantities arising from uncertainties in source activities and emission factors.

Typical levels of uncertainties in mobile and fixed source activities (e.g., number of vehicle miles traveled and number of units of fuel consumed) should be identified. Then, the typical uncertainties in emission factors (e.g., grams per mile of pollutant emitted per vehicle mile traveled and gram of pollutant per unit of fuel consumed) should be combined with the uncertainties in activities to produce net uncertainties in emissions. Finally, sensitivity studies should be carried out with urban diffusion models to assess the effect of these levels of uncertainties in source emissions on predicted concentrations.

Initial and Boundary Conditions

The initial condition for equation 5 is the concentration field at the time corresponding to the beginning of the simulation, $\bar{c}_i(x,y,z,0)$. Simulations are normally begun at sunrise, and the $\bar{c}_{i_0}$ field at that time is constructed from the station readings. A ground-level interpolation routine and assumptions regarding the vertical variation of the concentrations are required to generate the full $\bar{c}_{i_0}$ field from the station data. To minimize the effect of errors due to inaccurate initial conditions, one would like to simulate several days in succession, starting with a day at the beginning of which the concentrations are relatively low. Because readings are available from which to construct a $\bar{c}_{i_0}$ field, we do not expect a high level of uncertainty in the initial conditions when a previous time is simulated.

The boundary conditions for equation 5 consist of the concentrations upwind of the region, the pollutant fluxes at the ground (the source emissions), and the flux condition at the upper vertical boundary of the region. Concentrations upwind of the modeling region can be estimated if monitoring stations exist at the upwind edge of the airshed. In such a case uncertainties in these concentrations will be low when a previous time is simulated. The major source of uncertainty in boundary conditions generally arises at the upper vertical boundary. First, the temperature structure, for example, the height of the base of an elevated inversion layer, is not known precisely. Second, the pollutant flux condition at the boundary is also not known precisely.

Thus, the major uncertainty in boundary conditions when past time periods are simulated is in specifying the upper vertical boundary conditions, both the location of the boundary and the species flux condition at the boundary. Sensitivity studies should be carried out on the location of an upper boundary of no flux (an inversion base) to determine the effect of uncertainties in inversion base height on predicted concentrations.

A special problem arises in specifying initial and boundary conditions when a model is to be exercised under hypothetical emission conditions, for example, when the effect of emission control strategies is studied. Initial concentrations at sunrise, say, reflect nighttime emissions as well as, perhaps, the previous day's concentration levels if the airshed is not thoroughly flushed at night. For an inert pollutant such as CO it is reasonable to assume that initial and boundary concentrations under future conditions will reduce in direct proportion to emission reductions with account taken of the background levels (the rollback assumption). Although hydrocarbons are reactive, their initial and boundary levels can also be assumed to vary in direct proportion to emissions. The problem arises when NO_x and O_3 are considered. Two approaches to specifying initial and boundary conditions for NO, NO_2, and O_3 were developed by Reynolds and Seinfeld (27).

1. The first method of calculation is based on the assumption that NO and NO_2 concentrations at sunrise and at the boundaries of the airshed will be reduced from the base-year values in direct proportion to the reduction in total NO_x emissions, i.e.,

$$[NO] = \phi_{NO_x}[NO]_b$$

$$[NO_2] = \phi_{NO_x}[NO_2]_B$$

where ϕ_{NO_x} is the fractional reduction in NO_x emissions from the base year, and B denotes base-year values. Assuming a photostationary state for O_3 concentration (24),

$$[O_3] \sim \frac{[NO_2]}{[NO]}$$

we see that $[O_3]$ concentrations will remain the same as in the base year since the ratio of $[NO_2]$ to $[NO]$ remains the same.

2. The second approach for specifying the NO, NO_2, and O_3 initial and boundary condition is suggested by the rollback concept, in which O_3 concentrations are assumed to be proportional to hydrocarbon emissions and total NO_x concentrations are assumed to be proportional to NO_x emissions. These assumptions lead to the following expressions for future-year concentrations:

$$\frac{[NO] + [NO_2]}{[NO]_B + [NO_2]_B} = \phi_{NO_x}$$

$$\frac{[NO_2]/[NO]}{[NO_2]_B/[NO]_B} = \phi_{HC}$$

where ϕ_{HC} is the fractional reduction in hydrocarbon emissions relative to the base year.

Additional study should be directed to the problem of specifying initial and boundary conditions for emission control exercises.

SUMMARY

This paper discusses the concepts of validity and accuracy for air pollutant model calculations and suggests a number of numerical experiments that should be carried out on an urban diffusion model to test its validity and accuracy. These studies are summarized as follows:

1. Perform diffusion experiment in numerical turbulence field and compare data with conventional air pollution models using eddy diffusivities (17, and work in progress by Lamb);
2. Perform diffusion experiment for reactive species in numerical turbulence fields and compare data with conventional air pollution models with various reactive closure models (work in progress by Wengle and Seinfeld);
3. Perform sensitivity analysis of photochemical diffusion model to variations in meteorological parameters (21); and
4. Perform sensitivity analysis of photochemical diffusion model to variations in initial, boundary, and source concentrations (work in progress by McRae, Goodin, and Seinfeld).

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SURVEY OF STATISTICAL MODELS FOR OXIDANT AIR QUALITY PREDICTION

Leik N. Myrabo and Kent R. Wilson, Department of Chemistry and Energy Center, University of California, San Diego; and
John C. Trijonis, Transportation and Environmental Operations, TRW, Inc.

Oxidant air pollution is the result of a complex series of chemical reactions stemming from reactive hydrocarbon (RHC) and nitrogen oxide (NO_x) emissions. Transportation planning and other policies affect oxidant air quality by altering the spatial and temporal distribution of RHC and NO_x emissions. To evaluate the oxidant air quality impact of various policies requires that the relation between ambient oxidant levels and precursor emission levels be known. Attempts to determine this relation have followed 3 general approaches: smog chamber modeling, mathematical simulation of physical and chemical processes, and statistical-empirical models. Because of drawbacks in each of these approaches and because of the complexity of the photochemical smog process, considerable uncertainty still surrounds the relation between ambient oxidant concentrations and precursor emission levels.

Smog chamber models are based on the results of laboratory experiments wherein mixtures of RHC and NO_x are irradiated by sunlight to produce oxidant. By altering the amounts of RHC and NO_x in these experiments, one can gain information on the dependence of oxidant on precursor levels. Smog chambers have provided much of the basic understanding we have of photochemical air pollution. However, their use in air quality planning has uncertainties because of questions concerning how representative smog chambers are of real atmospheric conditions. In smog chambers, simulating real meteorology is difficult, and the hydrocarbon mix may differ from that in the real atmosphere. Also, wall effects in smog chambers produce effects that are absent in real atmospheres and conversely do not reproduce real effects of terrestrial surfaces. In addition, smog chamber results do not simulate the spatial distribution of emissions in a region.

The second approach, deterministic or mechanistic modeling of chemical and meteorological processes, involves mathematical simulation of emission patterns, diffusion and mixing, transport, and atmospheric chemistry. This deterministic type of model could in principle be an ideal planning tool since it can explicitly account for changes in the spatial and temporal distribution of emissions as well as changes in overall emission levels and meteorological variability. Much work has been done in developing and testing chemical-meteorological models, but serious questions still exist concerning the accuracy of such models in predicting the impact of future emission changes. These questions stem from the lack of sufficient understanding of turbulent mixing and diffusion, from uncertain knowledge of the reaction rates for atmospheric reactions, and from inadequacies in the available meteorological data. The application of chemical-meteorological models may also be limited by the expense associated with the extensive data base and the computer time required to run them.

The third approach, statistical-empirical modeling, centers on the use of actual atmospheric monitoring data. The relation between oxidant and precursors or oxidant and meteorological variables is derived from aerometric data by statistical analysis and simplifying physical assumptions. Empirical models benefit from the basic advantage that the influences of all the complex atmospheric processes are inherent in the aerometric data base, which forms the foundation of these models. Empirical models are also relatively inexpensive to develop and simple to apply. A disadvantage of the empirical approach is inaccuracy or sparsity or both of the required aerometric data. Since the models are developed from examining a particular range of real conditions, there is always a danger in extending the conclusions of such a model beyond the range of the data on which it was calibrated. Most (but not all) empirical models, for example, involve the assumption that the spatial distribution of emissions remains fixed and are not geared toward the assessment of the effects of alternative source sitings.

The purpose of this paper is to review the present state of the third approach to oxidant modeling: the statistical-empirical approach. In the interests of brevity, we will restrict our scope mainly to statistical-empirical models that have been used in a predictive capacity, not just to draw correlations. Thus, we will neglect a large part of the important statistical work that has been done on the correlations among meteorological and pollutant variables, for example, in the analysis of past air quality trends. In addition, we will restrict our review only to those models that have been applied to oxidant prediction, even though the methodology used to predict other pollutants can often be applied to oxidant as well.

Two classes of models for oxidant levels are reviewed; both have quite different aims. The first is short-term forecasting, with the goal of episode control. The basic relation is the variation of oxidant level with meteorological parameters. The hope is to predict episodes with enough lead time (hours to days) so that temporary emission controls can be applied to lessen the severity of the episode, or at least to provide health warnings. The second class of models has the goal of predicting the long-term effect of control strategies. The basic relation is that between emission levels and oxidant level. The hope is to evaluate and optimize long-term control strategies before implementation.

Before proceeding to survey statistical-empirical oxidant models, we should note that all models, including smog chamber and chemical-meteorological models, are in part statistical and empirical. Smog chamber and chemical-meteorological models also in reality depend on atmospheric data for calibration before they are used for predictive purposes. As defined here, statistical-empirical models are those that rely on aerometric data to determine the actual form of the oxidant-meteorological or the oxidant-precursor dependence.

SHORT-TERM PREDICTION (EPISODE CONTROL)

If one could predict far enough in advance that an episode of high air pollution level were going to occur, one could then try to reduce the seriousness of the episode by short-term control of emissions, for example, from traffic and particular industries, during the episode period. In addition, health warnings could be issued to advise sensitive individuals of when and where they should take particular precautions. Thus, based on measured pollutant and meteorological variables, several modeling efforts have used statistical-empirical techniques to try to predict air pollution levels hours or days in advance. For example, one might derive a relation statistically linking tomorrow's hourly maximum oxidant level to today's oxidant level, wind speed, inversion height, and temperature.

Three basic types of statistical approaches have been used to try to make predictions on this short-term scale: time series, multiple regression, and pattern recognition. For an introduction to the field (really a preview rather than a review, since this area until now has been characterized more by discussion than by in-depth studies), the reader should review the proceedings of the Conference on Forecasting Air Pollution (6) and, perhaps for background, the proceedings of the Symposium on Statistical Aspects of Air Quality (23).

Time Series

Pollutant monitoring data can be considered as a sequence of observations, a time series of pollutant measurements $z_1, z_2, \dots, z_n$ at times 1, 2, . . . , n. One wishes, knowing n values, to predict the next ℓ values. One can use just the previous values of the time series itself to predict the future values, a univariate time series (e.g., past oxidant measurements to predict future oxidant measurements), or one can use a multivariate time series and in addition consider other predictor variables such as meteorological measurements.

As explained by Box and Jenkins (3), one can set up a general form of linear stochastic model of a univariate time series as

$$w_t - \varphi_1 w_{t-1} - \dots - \varphi_p w_{t-p} = a_t - \theta_1 a_{t-1} - \dots - \theta_q a_{t-q} \tag{1}$$

where $w_t = \nabla^d z_t$, ∇ being the backward difference operator; and $\nabla z_t = z_{t-1}$, which may be repeated d times. Pollutant time series that contain daily, weekly, or yearly seasonality may be handled by using ∇_s, where $\nabla_s z_t = z_t - z_{t-s}$; for example, for daily measurements with a weekly cycle, s = 7. Fitting a model to the time series involves deciding how many times to difference with ∇ (to achieve a stationary time series), choosing how many parameters $\varphi_1, \dots, \varphi_p$ and $\theta_1, \dots, \theta_q$ to include, and then adjusting them to obtain optimal forecasts. Diagnostic checking of the model involves examining the residuals $a_t, a_{t-1}, \dots, a_{t-q}$ that relate w_t to past values $w_{t-1}, \dots, w_{t-p}$. These residuals represent all factors other than the past values w_{t-1}, w_{t-2}, and so on that actually determine the values of the time series. If the model fits the time series well, the residuals should behave nearly like white noise, being a series of normally distributed random values with mean zero. Since the expected value of the residuals is zero, forecasts of future values of the time series, i.e., future pollutant values, can be made by setting to zero the unknown residuals yet to come.

Work along these lines has been carried out by Box and Tiao and coworkers at the University of Wisconsin, by McCollister and Wilson at the University of California, San Diego (27), and by Chock and Terrell at General Motors Research Laboratories (10).

Some results of the work by McCollister and Wilson are shown in Figure 1 for univariate oxidant prediction both of daily instantaneous oxidant maxima and of hourly oxidant values. All forecasts are made by using data before 10 a.m. the day before the day being forecast. Persistence assumes the day being forecast will be the same as the previous days; LAAPCD is the prediction of the Los Angeles Air Pollution Control District from pollutant and meteorological data, and model is a Box-Jenkins univariate time series with 2-step ahead prediction. Such a univariate time series model that predicts future oxidant values solely on the basis of past oxidant values does a bit better than persistence (which assumes the future mimics the past exactly) and, surprisingly, even a bit better than predictions made by trained meteorologists using both meteorological and pollutant data. All 3 methods, however, have fairly large average errors, in the 35 to 50 percent range, perhaps too large for actual health warning or short-term emission control usage. McCollister and Wilson have also developed multivariate time series oxidant forecasts using multivariate time series of meteorological variables.

Chock and Terrell (10) have applied both univariate and multivariate time series techniques to weekly average daily maximum oxidant data. Figure 2 shows a comparison of their various time series studies as applied to weekly 1970 oxidant data. The results shown are for long-term prediction, using the previous years' oxidant data, and could be improved by using oxidant data up to the week to be predicted. Little predictive information was found in week-old meteorological data, as might be expected from weather forecasting experience (6). Thus, their multivariate predictions use future and not past meteorological data (radiation intensity, wind speed, and dry bulb temperature). Although the weekly time span used is probably too long for episode control or short-term health warnings, these same techniques demonstrated by Chock and Terrell could also be applied to daily or hourly data.

Work is in progress at the San Francisco Bay Area Air Pollution Control District on both univariate and multivariate time series techniques as applied to oxidant data.

Figure 1. Comparison of forecasts of daily instantaneous oxidant maxima for 1972 by 3 methods for Los Angeles County monitoring stations.

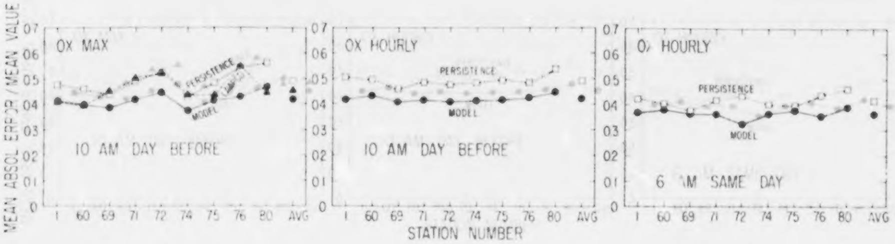
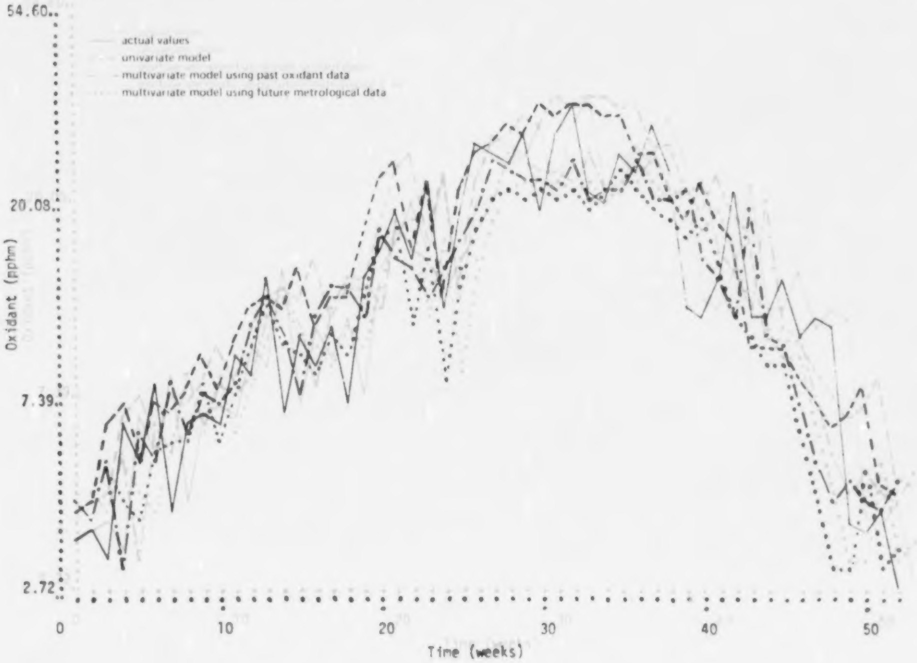


Figure 2. Various time series predictions of 1970 weekly average daily hourly maximum oxidant concentrations (log scale) at Riverside, California.



In addition, studies have been carried out there in which a canonical correlation method (19) is used, which is essentially a regression on the univariate oxidant time series and thus is somewhat related both to Box-Jenkins time series analysis and to multiple regression.

There are also other studies that have aims different from short-term forecasting. These studies, in which time series techniques have been applied to oxidant data, include work by Merz, Painter, and Ryason (29); Lee, Sarin, and Wang (24); Tiao, Box, and Hamming (36); and Box and Tiao (4, 5). Much of the mathematical approach used in these studies is also applicable to short-term oxidant forecasting.

Multiple Regression

Many different measured variables might be used as predictors to forecast oxidant values far enough ahead for short-term controls on emissions to be implemented or for health warnings to be issued: pollutant concentrations (CO, SO_2, RHC, NO, NO_2, oxidant), local meteorological variables (wind vectors, inversion heights, temperatures, solar radiation, relative humidity, precipitation, cloud cover, barometric pressure), and more distant meteorological variables (upper air data, surface meteorology outside the air basin). Multiple regression (15) has been an approach taken by several authors—the linear combination of these predictor variables X_i that best forecasts oxidant levels,

$$\mathrm{Ox} = \alpha_0 + \Sigma_i \alpha_i X_i + \epsilon \qquad (2)$$

in which α_0, α_1, . . . are constants to be discovered and ϵ is an error term.

Charles Bennett (2) used stepwise multiple regression to relate maximum hourly average oxidant at several Los Angeles area stations to (a) yesterday's maximum hourly oxidant at the given station, (b) highest hourly NO_2 concentration observed between 6 and 9 a.m. today at the downtown Los Angeles station, (c) the 24-hour height change at 500 mb (5 MPa) based on the 4 a.m. atmospheric soundings above Vandenberg Air Force Base, and (d) the 850-mb (85-MPa) temperature based on the 4 a.m. sounding above Los Angeles Airport. For 4 stations, the correlation coefficients between this afternoon's predicted and measured maximum hourly concentrations ranged from 0.69 to 0.77 during the June-September 1973 and 1974 periods. Stratifying the data by weekends and weekdays further improved the fit, and the tendency to underpredict higher values was reduced by weighting high oxidant days. A comparison of observed and predicted values (with the above refinements) is shown in Figure 3.

Chock and Terrell (10) applied multiple regression to predict weekly averages of maximum daily oxidant from concurrent weekly average weather parameters, first using a regression analysis to screen out the best subset of independent predictors, which were found to be radiation intensity, wind speed, and dry bulb temperature. (These weather parameters were then also used for their multivariate weekly time series analysis.) Regression in terms of logarithms of the variables was found to be useful. The coefficients of determination, R^2, the fraction of the total variation about the mean explained by the regression, ranged from 0.79 to 0.84 for various models with and without previous oxidant data as a predictor. These R^2 values are to be compared with the 1-week ahead forecast values obtained by Chock and Terrell of 0.71 for univariate weekly oxidant time series and 0.82 for multivariate weekly time series using concurrent meteorological data.

Tiao, Phadke, and Box (37) used a regression model on logarithmic data from Los Angeles to derive a forecasting relation for daily maximum hourly oxidant based on the previous day's oxidant value, month of the year, 4 a.m. NO_2 level, 4 a.m. inversion base height and its square, difference between the inversion breaking temperature and the 4 a.m. surface temperature, and the average 1 to 4 a.m. wind speed. The variance of the error was significantly reduced by introducing the early morning NO_2 and meteorological data.

Bruntz, Cleveland, Kleiner, and Warner (7) fitted a regression for New York data relating log of ozone plus a constant from 1 to 4 p.m. to logs of 4 predictor variables: morning average wind speed, solar radiation, maximum daily temperature, and mixing height. The meteorological and ozone data are in part concurrent. The correlation coefficient between predicted and fitted $\log_{10}$ (ozone + 5 ppb) is 0.84 and is little affected by omitting mixing height from the regression equation.

An interesting application of an approximate nonlinear regression, with aspects of pattern recognition, is the point classification system for ozone prediction developed by Zeldin and Thomas (39) of the San Bernardino County Air Pollution Control District in California. Six classification categories are defined: stability, 950-mb (95-MPa) temperature, inversion base height, coast to desert pressure gradient, day of the week, and month of the year. Points are assigned separately to each of the 10 classes into which each category is divided, and the sum of the number of points over all categories is equated to the predicted peak ozone level. The model, once calibrated, is thus based entirely on meteorological predictors and not on previous ozone levels. For this reason, it can be used to correct monthly or yearly ozone data for the effect of meteorological variability, to allow an approximate removal of meteorological effects from the trends of pollution levels with changing emissions, and, it is hoped, to provide more reliable reflection of the real effects of long-term control strategies.

Pattern Recognition

There is no a priori reason to suppose that the relation of oxidant to meteorological and pollutant predictors should be best fitted by any particular mathematical scheme. More general methods for forecasting exist than either the usual time series or multiple regression techniques discussed above. Groups at Technology Service Corporation (6), at Environmental Research and Technology (6), and at the University of Washington and the University of California, San Diego, have done explanatory work in applying formal pattern recognition techniques (28) to air pollution; to our knowledge, no full treatment has yet been published. Several other studies, however, involve stratification and classification techniques that at least share something of the viewpoint of pattern recognition, and Pollack (32) has discussed some of the possibilities.

Two basic tasks are involved. First, out of the large set of possible predictors, a smaller number of significant features must be selected, the aim being to find those that singly or in combination can best be used to forecast future oxidant levels. These features may themselves be functions of several members of the original predictor set and may include the output of time series and multiple regression forecasts. Various formal techniques exist for such feature extraction and ranking (28); but, since the possible number of features is infinite, good judgment is also helpful. The object is to find a small set of features that contain most of the information of the larger predictor data set. Too many features degrade performance by introducing additional noise and by adding complication and expense to the computations. Too few features result in loss of information and prediction accuracy.

The second task is to find an optimal forecasting method linking these features to oxidant values. Again many formal techniques exist (28). Multivariate piecewise linear regression could be used to approximate global nonlinearities in the "real" feature-oxidant relation yet still give continual predictions. If prediction into categories is desired, for example, whether a given day will or will not exceed a particular oxidant standard, then many pattern classification methods (28) are available.

An example of an approach that is in the spirit of pattern recognition, but does not use its formal mathematical methodology, is the objective ozone forecast system developed by Davidson (13) to predict the occurrence of days from July through October with ozone levels equal to or greater than 0.35 ppm. The forecasts are based on meteorological data available by 9 a.m. The forecaster first classifies days into 3 patterns, as shown in Figure 4, by 2 features: the 24-hour 500-mb (50-MPa) height change at Vandenberg Air Force Base and the 6 a.m. 2,500-ft (750-m) temperature at Los Angeles Airport. If the feature values for that day lie in area A of Figure 4, the forecast is <0.35 ppm oxidant; if they lie in area C, the forecast is ≥ 0.35 ppm. If the feature values lie in the intermediate area B, then other features are called into play for discrimination: first, the differences in 7 a.m. pressure and temperature between the Los Angeles (coastal) and Palmdale (inland) airports and, if necessary, the 8 a.m. visibility at Los Angeles Airport and the surface temperature change during an hour period at Palmdale. The accuracy of the forecasts is shown by the following tabulation of the results of 815 forecasts from July to October, 1964 to 1971.

	Actual	
Predicted	<0.35	≥0.35
<0.35	Correct 484	Incorrect 29
≥0.35	Incorrect 94	Correct 208

The skill score of the 815 trials was 0.66, according to Davidson's definition of a skill score:

$$S = \frac{R - E}{T - E} \tag{3}$$

where

R = number of correct forecasts,
T = total number of forecasts, and
E = number of forecasts expected to be correct due to chance.

In addition to Davidson's work, others have also developed stratification schemes that can be used in oxidant forecasting. For example, in recent work Bruntz et al. (8) related oxidant levels in New York and New Jersey to wind speed and solar radiation and Tiao, Phadke, and Box (37) studied the meteorological conditions when the daily instantaneous peak oxidant exceeded the 0.50-ppm alert level in Los Angeles County.

LONG-TERM MODELS (LONG-TERM STRATEGY)

The purpose of long-term air quality models is to predict the air quality impact of long-term changes in emission levels. These emission changes result from the growth or attrition of present sources, from control strategies, and from new developments (such as highways). Long-term oxidant models are specifically concerned with the effects of the level and spatial-temporal distribution of reactive hydrocarbon and nitrogen oxide emissions.

Four types of long-term statistical-empirical models are reviewed below. The first, linear rollback, is the most simplistic. Slightly more complex are modified rollback models based on empirical relations observed between maximum oxidant levels and hydrocarbons in the atmosphere. The third type of model is based on empirical relations of oxidant to both HC and NO_x. Each of the first 3 types neglects the spatial-temporal distribution of emissions; accordingly, each is restricted to analysis of the impacts of regionwide changes in the total level of emissions. The fourth type of empirical model illustrates how the spatial distribution of emissions can be incorporated into the statistical approach.

Linear Rollback

The linear rollback model for oxidant is based on the rather arbitrary assumption that maximum hourly oxidant levels in a region are directly proportional to total reactive hydrocarbon emissions in that region (12, 14). The model is calibrated by using aerometric data for oxidant as well as emission estimates for reactive hydrocarbons in some "base" year. Stated mathematically, the linear rollback relation between maximum hourly oxidant OX and regionwide reactive hydrocarbon emissions is

$$OX = \frac{RHC}{RHC^{\circ}} OX^{\circ} \qquad (4)$$

where

OX° = maximum hourly oxidant measured in the base year, and
RHC° = total reactive hudrocarbon emissions in the base year.

Actually, the linear rollback model is not a statistical-empirical oxidant model because the relation is based on an arbitrary assumption rather than on an analysis of aerometric data. As with all types of models, linear rollback is calibrated with atmospheric measurements; however, the relation itself is not based on atmospheric observations. We include the linear rollback model in this discussion because it is similar to most statistical-empirical models in its simplicity of application and because it has been so widely used in air quality planning.

The defects of the linear rollback model are many. Linear rollback relates oxidant to hydrocarbons only; yet, it is known that oxidant levels depend significantly on both RHC and NO_x emissions. Linear rollback neglects important nonlinearities in the oxidant-hydrocarbon relation; the existence of these nonlinearities has been demonstrated by smog chamber, aerometric, and theoretical studies. Linear rollback also neglects background oxidant levels that may be significant, especially if the model is applied to determine oxidant concentrations near the federal standard.

In the form presented above, the linear rollback model also suffers from errors introduced by meteorological variance in the aerometric calibration data. Rather than calibrate the model with the actually measured maximum hourly oxidant level, it would be more appropriate to perform a statistical analysis of the base-year aerometric data. A statistical analysis of the data can determine the "expected" maximum hourly oxidant, which may differ significantly from the actually measured value (30). By determining the "expected value" from a statistical analysis, the model can at least be calibrated to predict a statistically well-defined parameter.

Aerometric Relation of Oxidant to HC

A second approach that relates maximum oxidant to reactive hydrocarbon emissions is modified rollback. Unlike linear rollback, modified rollback is based on a statistical relation between oxidant and hydrocarbons. This relation is usually in the form of upper limit curves determined from atmospheric data. Like linear rollback, the modified rollback approach can be applied only to regionwide problems since the spatial distribution of emissions is neglected.

The most widely used modified rollback model is the EPA Appendix J approach (17, 18, 34). The curve shown in Figure 5 represents the upper limit of maximum hourly oxidant levels that are associated with various concentrations of 6 to 9 a.m. nonmethane hydrocarbons (NMHC). The maximum daily oxidant levels and early morning hydrocarbon levels have been measured at the same location. Data have been used from 5 cities for the period from 1966 to 1968.

The modified rollback analysis is as follows: For a given base year, the measured maximum hourly oxidant level is plotted at point A°. The curve is then used to characterize a base year NMHC level at B°. For a new reactive hydrocarbon emission level, a new NMHC level is characterized at B, where the ratio of B to B° is in direct proportion to the ratio of the new and base-year emission levels. The curve is then used to predict an oxidant level, A, corresponding to the new emission level.

The EPA Appendix J modified rollback model has several serious limitations. The following are the main sources of error.

1. The model is subject to inaccuracies in the aerometric data base for oxidant and hydrocarbons.

Figure 3. Comparison of observed oxidant levels with Bennett's predictions using stepwise multiple regression.

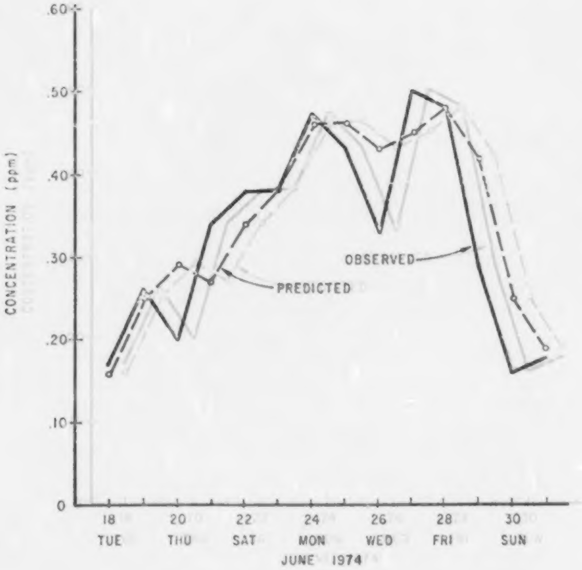


Figure 4. Davidson's initial decision rule for determining whether oxidant will reach the 0.35-ppm level.

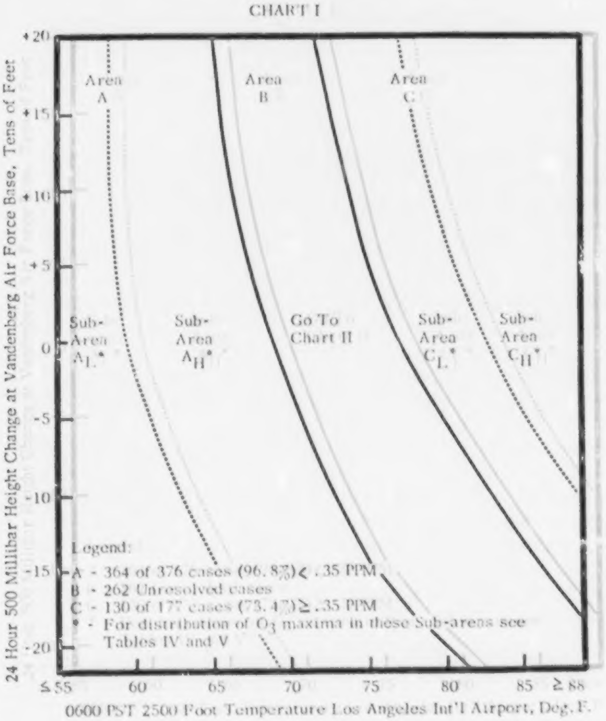
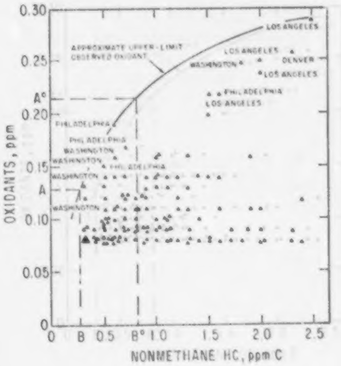


Figure 5. Maximum daily hourly average oxidant as a function of 6 to 9 a.m. average NMHC at stations throughout the country.



2. The role of NO_x in oxidant formation is neglected. The upper limit curves may no longer be appropriate if the HC-NO_x emission ratio is altered.
3. Relating oxidant concentrations to 6 to 9 a.m. precursor concentrations neglects the role of post 9 a.m. emission in oxidant production.
4. The approach does not account for transport. Early morning precursor and afternoon oxidant measurements at one location are likely to be associated with 2 different air masses.
5. The effect of meteorological variables is not taken into account. The observed relation of maximum oxidant to hydrocarbons may be spurious in the sense that it may be due to a mutual correlation with meteorological variables.
6. The upper limit curves are not defined in a statistically meaningful manner. Likewise, the calculation of degree of control required neglects statistical considerations.
7. Background HC and background OX contributions are neglected.

In addition, since the oxidant values shown in Figure 5 reach only 0.3 ppm, the EPA Appendix J approach cannot be used for regions that currently experience maximum oxidant levels greater than 0.3 ppm.

Schuck and Papetti of EPA have specialized and improved the modified rollback approach for the Los Angeles area (35). Their model is based on Figure 6, which gives the upper limit of maximum daily oxidant levels measured anywhere in the Los Angeles basin as a function of 6 to 9 a.m. hydrocarbons averaged over 8 stations in the basin. Figure 6 is based on data for 1971. The application of the Schuck and Papetti curve directly parallels the procedure for the EPA Appendix J curve.

The Schuck and Papetti model has the advantage of being specific to the region in which it is applied. Also, it accounts for transport in an approximate way by including all the monitoring stations in the air basin simultaneously. However, the other limitations of the EPA Appendix J approach (e.g., errors in the aerometric data, neglect of NO_x, neglect of post 9 a.m. emissions, neglect of meteorology, and the lack of statistical treatment) are shared by the Los Angeles upper limit curve.

Aerometric Relations of Oxidant to HC and NO_x

Several investigators have formulated statistical-empirical models that relate oxidant to both HC and NO_x. Nearly all applications have been restricted to the Los Angeles area because of the relative abundance of aerometric data in that area. As with the previously discussed models, these empirical models are restricted to the analysis of regionwide emission changes.

Merz, Painter, and Ryason (29) of Chevron Research Corporation used regression analysis to examine the relation between oxidant and early morning precursor levels at downtown Los Angeles. They regressed maximum daily 1-hour oxidant against 6 to 9 a.m. concentrations of NO_x and total hydrocarbons (THC). To minimize meteorological variations and, therefore, to minimize spurious oxidant-precursor dependencies due to mutual interrelations with meteorological variables, they entered data only for August, September, and October. The results of their regression analysis are shown in Figure 7.

The simple log-linear regression used by Merz, Painter, and Ryason indicated that NO_x reductions would have a slight but beneficial impact on oxidant air quality. This is in contrast to the results of the 2 models that follow in this discussion. The next 2 models indicate that NO_x emission reductions may have an adverse effect on oxidant air quality.

The Chevron research model can be used to predict the impact of regionwide changes in emission levels by proportioning the atmospheric concentrations of HC and NO_x to the changes in the respective emission levels. The improvements of the Chevron research model over the modified rollback models based on upper limit relations of OX to HC are the inclusion of NO_x and a better statistical treatment. However, the Chevron research model shares many limitations with the previous models: inaccuracies in the data base, neglect of post 9 a.m. emissions, neglect of transport, and neglect of background contributions.

Kinosian and Paskind (22) of the California Air Resources Board examined the relation between oxidant and precursors at 4 locations in the metropolitan Los Angeles air quality control region. They used ambient data for 6 to 9 a.m. THC and NO_x concentrations and for maximum hourly oxidant concentrations measured at the same station. The data base consisted of measurements for July through September from 1969 to 1972. THC measurements were converted to NMHC estimates by using correlations established between THC and NMHC at 2 Los Angeles monitoring sites.

At each location, the data were grouped according to various early morning HC concentrations. For each HC level, a regression was run between oxidant levels and NO_x concentrations. The resulting curves, giving expected oxidant levels as functions of early morning HC and NO_x concentrations, are shown in Figure 8.

The Kinosian and Paskind results can be used to predict the impact of emission level changes in the same way as the Chevron research model. The limitations in using the Kinosian and Paskind results are the same as in using the Chevron research results.

Trijonis (38) used a stochastic model to examine the relation of oxidant levels in central Los Angeles to HC and NO_x emission levels. For given HC and NO_x emission levels, he determined the joint distribution of morning HC and NO_x concentrations (7:30 to 9:30 a.m. averages) at downtown Los Angeles from 5 years of Los Angeles APCD monitoring data (1966 to 1970). He also determined the probability that midday oxidant would violate the state standard (0.10 ppm for 1 hour) as a function of the morning concentrations. For oxidant, an average was taken of maximum hourly values between 11 a.m. and 1 p.m. at downtown Los Angeles, Pasadena, and Burbank, weighted according to wind speed and direction, so that the maximum oxidant would correspond as closely as possible to that in the air mass that had been over downtown in the morning. The joint morning HC-NO_x distribution and the probability of a standard violation as a function of morning precursor levels were determined separately for summer and winter.

By assuming that the joint HC-NO_x distribution responds linearly to emissions and that the oxidant standard violation function remains constant as emission levels change, Trijonis calculated the expected number of days per year that midday oxidant in central Los Angeles would exceed the state standard as a function of HC and NO_x emission levels. Figure 9 shows the results.

The model used by Trijonis involves several limitations similar to those of the upper limit models: inaccuracies in the aerometric data, neglect of post 9 a.m. emissions, and neglect of background contributions. The improvements in the approach are the inclusion of NO_x, a better statistical treatment, and the allowances for pollutant transport.

Spatial Resolution

Many statistical approaches consider the air basin as a single point. Although greatly simplifying the development of a model, this approach is inadequate for land use and transportation planning, which practically must consider the geographical positioning of alternative sites and the spatial distribution of their effects. A key assumption for the validity of a point air basin model is that the spatial distribution of the emission sources remains constant. In contrast, one of the thrusts of a model for planning should be the evaluation of the effects of changes in this distribution. An additional problem with the use of a point air basin model lies in the practical implementation of an effective environmental review procedure. In reviewing a proposed source, the agency granting approval may not wish to allow a significant air quality deterioration as a result of the project. If, for example, a significant deterioration is defined as a 10 percent change in the index of air quality, a serious problem results. It is unlikely that any single source would result in a 10 percent increase in air quality index for a total air basin. By a lumped air basin evaluation, therefore, a source having a significant environmental impact would rarely be found, and the air quality element of an environmental review would be rendered ineffective. For these reasons, a group at the

Figure 6. Schuck and Papetti's aggregated upper limit curve for the metropolitan Los Angeles air quality control region.

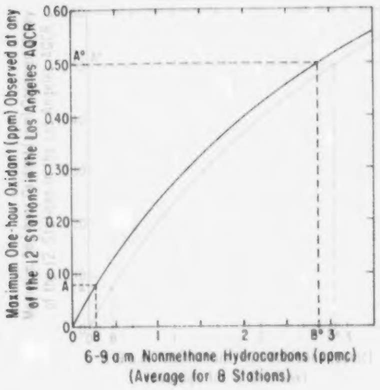


Figure 7. Merz, Painter, and Ryason's relation of NO_x and NMHC assumed as 50 percent of total HC and oxidant for downtown Los Angeles.

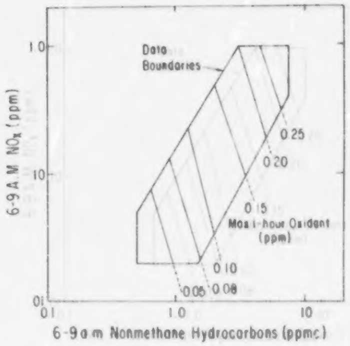


Figure 8. California Air Resources Board aerometric results, relation between 6 to 9 a.m. NO_x, 6 to 9 a.m. HC, and maximum hourly oxidant concentrations at selected sites (individual curves show total and NMHC concentrations in ppm).

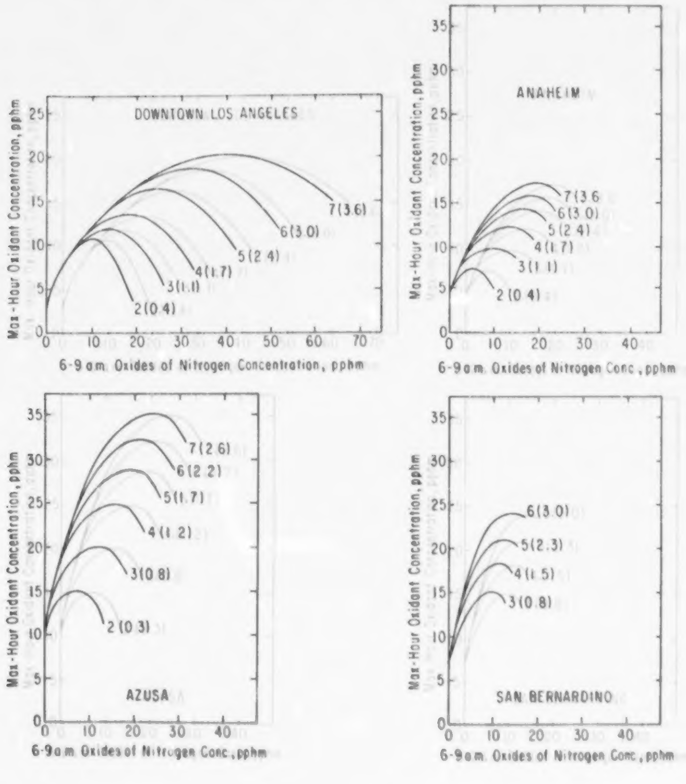


Figure 9. Expected number of days per year exceeding 0.10 ppm versus NO_x and RHC emissions levels for central Los Angeles.

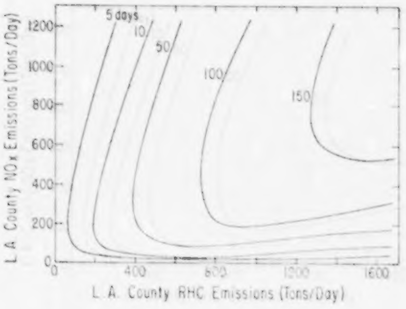
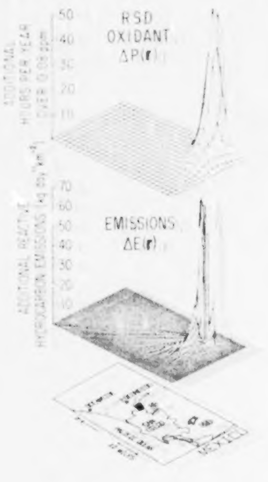


Figure 10. Application of spatially resolved model to predict effect on oxidant levels of a large regional development.



University of California, San Diego, has developed a statistical-empirical oxidant model with spatial resolution (31, 9).

Calibration of the relation between the spatially resolved emission function $E(\underline{r})$ and the resultant spatially resolved pollution function $P(\underline{r})$ is accomplished by using emissions and air quality data. Geocoded average daily RHC emission source functions $E(\underline{r})$ from mobile and stationary sources are calculated for Los Angeles and San Diego. $P(\underline{r})$ is expressed in terms of the number of hours per year higher than the federal 0.08-ppm oxidant standard. Data from 17 air quality monitoring stations in the San Diego and Los Angeles area are used in the calibration. The dependence of $P(\underline{r})$ on $E(\underline{r})$, averaged over meteorology $M(\underline{r})$, is approximated by integrating the RHC emissions picked up by seasonal prevailing windstream corridors from the ocean to each monitoring station and then by averaging over 4 seasons. The corridor width is chosen to be approximately a tenth of the maximum dimension of the Los Angeles and San Diego study areas.

A relation between hours per year higher than the federal standard and RHC picked up by the windstream is then developed by regression on the data from the 17 stations. This statistical relation may then be used to predict the spatial distribution of Ox resulting from a given spatial distribution of RHC emissions. An example of such a calibration is shown in Figure 10. The change in land use function $\Delta L(\underline{r})$ produces a change in the emission function $\Delta E(\underline{r})$, which is added to the base case emission function $E(\underline{r})$. The new total emission function is then used to calculate a new air quality function $P'(\underline{r})$, differing from the base case air quality function $P(\underline{r})$. The change in oxidant air quality resulting from altered land use $\Delta L(\underline{r})$ is $\Delta P(\underline{r}) = P'(\underline{r}) - P(\underline{r})$, in other words, the difference between air quality functions calculated with and without the development.

The model, like all existing oxidant models, has several limitations. Specifically, only RHC and not NO_x is considered. The windstreams used are only a crude representation of meteorological reality. The 17 data points on which the calibrating regression is based are quite noisy, and therefore the regression has a large uncertainty.

USEFULNESS OF STATISTICAL MODELS

Advantages

Statistical-empirical models have 2 major advantages. The first is their close relation to the actual atmospheric data on which they are based. Thus, we can hope to predict successfully even when deterministic understanding of the complex real world is incomplete. We can also hope that relations first inferred statistically may sometimes lead us in the end to a more fundamental understanding of the physical or chemical mechanism underlying the relation.

The second advantage is the relative simplicity and low cost of the development and use of statistical-empirical models. Computation using statistical-empirical models is usually rapid and relatively inexpensive. Thus, such models may be widely and repetitively applied, for example, to predict air quality each day at all monitoring stations in a region or to evaluate the air quality impact of large numbers of proposed land use and transportation projects.

Limitations and Dangers

That statistical-empirical models are derived from real atmospheric data is at once an advantage and a disadvantage. The disadvantage is that one is not assured of reliability in extrapolating the model beyond the range of conditions contained in the data from which it was derived. Since control strategies often are designed to drastically alter the present situation, one should be quite cautious in assessing the accuracy of such statistical predictions. One can make reliable error estimates for predicting tomorrow's oxidant level based on today's pollutant and meteorological measurements because tomorrow's meteorological pattern will probably be a repetition of the past. On the other hand, the probable error to be assigned to a prediction of the change in oxidant level due to an untried control strategy that would drastically change RHC and NO_x emissions is difficult to assess.

Short-term air quality forecasting has intrinsic limitations because air quality depends on meteorological variables that are themselves only imperfectly predictable (6). One should not expect to be able to predict air quality better than the weather. Certainly, unless there are major breakthroughs in weather forecasting, we cannot expect to predict short-term air quality more than a few days into the future any better than the mean value for the area in question at that time of year and time of day (and perhaps day of the week).

Caution should also be exercised in the use made of short-term predictions for episode control. One should not blindly assume that short-term emissions changes will always produce the obvious short-term results. For example, the evidence from both the east and the west coasts indicates that, although average precursor concentrations (RHC and NO_x) drop on weekends with altered emission patterns, the average oxidant level does not necessarily drop, and under some circumstances even rises (8, 11, 16, 20, 21, 25, 26, 33).

Suitable Areas for Application

The field of statistical-empirical oxidant modeling is in an early stage of development. Many obvious possibilities have not yet been tried, and imaginative new applications will certainly emerge. Several possible application areas are, however, already clear.

Short-Term Forecasting

1. Episode control. If one can predict air pollution episodes ahead of time, perhaps one can reduce their severity by altering the emission pattern through short-term

control of traffic and stationary sources.

2. Health warning. Whether one can control episodes, one can warn those particularly susceptible to air pollution effects to take precautions such as avoiding exercise, staying in filtered rooms, or leaving the area.

3. Crop protection. Perhaps with episode warnings, agricultural crops in some instances can be protected by spraying, irrigating, or covering.

Long-Term Prediction

1. Control strategy assessment. If one can assess the air quality impact of control strategies, one can optimize the benefit-cost ratio among control strategy options.

2. Regional planning. One can evaluate the air quality impact of alternative futures implied by different regional plans.

3. Transportation planning. The air quality impact of alternative transportation plans, for example, mode-split variations, can be assessed.

4. Environmental impact reports. Given a statistical model with spatial resolution, one can assess the air quality impact of highways, airports, industrial and commercial centers, and new towns. The impact can in theory at least be predicted as a function of location of the emission source and location of the receptor.

CONCLUSION

Statistical-empirical modeling of oxidant levels is currently proceeding in 2 directions, each dictated by the prediction time span and the envisioned use. The first direction is short-term oxidant forecasting over the range of hours to days, with the goal of episode control by short-term emission control as well as the issuance of health and perhaps agricultural warnings. The major tools being used are Box-Jenkins time series analysis, multiple regression, and aspects of pattern recognition.

The second direction is long-term prediction over the scale of years of the expected changes in oxidant levels due to changes in RHC and NO_x emissions, either aggregated for an air basin or more rarely spatially resolved. The goal of such prediction is the assessment of the probable effects on oxidant air quality of various emission control strategies. Possible applications include optimization of control strategies, regional planning, transportation planning, and environmental impact reports. The major categories of models are rollback, prediction from HC, prediction from HC and NO_x, and spatial resolution. The advantages of using statistical-empirical models include (a) their close relation to the actual air measurement data from which they are derived, allowing the possibility of correct prediction even in the absence of complete understanding of the underlying phenomenon, and (b) their usual simplicity and low cost of development and use.

Their disadvantages and dangers include uncertain reliability outside the range of the data used in calibration, inability to predict short-term levels better than the associated weather features, and danger of assuming that short-term emission changes will always produce the expected result.

Oxidant modeling and prediction of all varieties are still an uncertain art that is in the early stages of development, and for this reason it is often wise to evaluate the same question by using a variety of modeling approaches. No aspect of the field is yet mature or free from difficulties. Chemical modeling in a smog chamber is on too small a scale and has too great differences from conditions of the real atmosphere. Mechanistic modeling of chemistry and meteorology has too many unknowns for the state of our chemical and meteorological understanding as well as for our computational capacity. Statistical-empirical modeling is most often called on to perform tasks that carry it into statistically shaky ground: (a) short-term prediction of extreme values, episodes on the tail of the distribution that are not representative of the data set as a whole on which the model is based and (b) long-term prediction of what would happen under control strategies that would alter the emission pattern far beyond the situation that produced the data used to derive the model.

Yet, uncertainty is no excuse for inaction. We can set reasonable bounds with a variety of prediction schemes. Although the numerical uncertainties may be large, the direction in which to proceed in controlling air pollution is usually clear. We can climb up a hill without knowing precisely how far it is to the top, and, as we proceed, the view of the top becomes clearer.

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RURAL OXIDANT AND OXIDANT TRANSPORT

R. M. Angus and E. L. Martinez, Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina

Before 1970, surface measurements of oxidants in rural areas were made infrequently and did not indicate the presence of particularly high concentrations (1,2). But in the course of a study conducted by the U.S. Environmental Protection Agency in 1970 (3), investigators found oxidant concentrations in a rural area of western Maryland and eastern West Virginia that frequently exceeded the present national ambient air quality standard (NAAQS) of 160 μg/m³ (0.08 ppm) for a 1-hour average. Although the NAAQS is for photochemical oxidants, the measurement method prescribed is specific for ozone. Simultaneous oxidant and ozone specific measurements by Richter (4) during part of the 1970 study showed that virtually all of the oxidants measured were ozone. Follow-up studies of increasing magnitude were sponsored by EPA and were conducted in 1972, 1973, and 1974 (5,6,7). The extensive measurements carried out in the summer of 1974 were made at widely separated sites in the eastern Midwest.

The studies showed that the oxidant standard was exceeded on a significant number of days at both urban and rural sites. The rural sites exceeded the standard more often than urban sites and higher maximum concentrations were measured at the rural locations. Table 1 (7) gives data on maximum ozone observed and frequency of ozone above the standard 160 μg/m³ (0.08 ppm) for the monitoring locations shown in Figure 1. At DuBois, a small city in rural Pennsylvania, the oxidant standard was exceeded 341 hours during the period from June 14 to August 31, 1974. During the same period at Pittsburg, approximately 160 km (100 miles) southwest of DuBois, the standard was exceeded only 106 hours. The maximum hourly concentration measured at DuBois was 400 μg/m³ (0.20 ppm); at Pittsburgh it was 280 μg/m³ (0.14 ppm). Similar high values of ozone have also been measured in rural areas of New York (8,9), New Jersey (10), Wisconsin, and Florida (12). Thus, in many areas of the eastern United States, high concentrations of oxidants are found in both rural and urban areas.

SOURCES OF RURAL OXIDANTS

Several possible sources of rural oxidants must be considered in efforts to account for the observed concentrations. These sources include the large quantities of man-made precursors that are emitted in urban areas and that may move into rural areas while reacting to form oxidants and also the oxidants formed from man-made precursors that originate in the nonurban areas. The precursors are the nitrogen oxides and organic compounds that react to form oxidants in the presence of sunlight. The principal sources of organic compounds are the hydrocarbon emissions from automobile and truck exhausts, gasoline vapors, paint solvent evaporation, open burning, dry cleaning, and industrial operations. Nitrogen oxides are emitted primarily from combustion sources, such as electric power generation units, gas- and oil-fired space heaters, and automobile, diesel, and jet engines. There are also 2 possible natural sources of surface level oxidants: (a) downward transport from the ozone-rich layers in the stratosphere into the lower troposphere near the surface and (b) photochemical generation from hydrocarbons emitted by vegetation. The available evidence strongly indicates that frequent and persistent concentrations of ozone near the surface above 160 μg/m³ (0.08 ppm) are not caused solely by natural sources and that the background that can be attributed to natural sources is usually 80 to 100 μg/m³ (0.04 to 0.05 ppm).

The amount of ozone transported from the stratosphere may be estimated from the numerous vertical ozone soundings of the atmosphere made in past years (13). These generally show ozone concentrations occurring at a maximum in the lower stratosphere, decreasing to low levels at or near the tropopause, and slightly decreasing toward the surface. Ozone levels near the surface that appear to be largely of stratospheric origin may at times range from 60 to 100 μg/m³ (0.03 to 0.05 ppm) (15). Temporary higher readings, however, are possible with unusually deep and vigorous vertical mixing induced by strong cold fronts, jet streams, thunderstorms, or some combination of these. These are sporadic, usually short-lived events, lasting on the order of minutes or, less often, a few hours. Lightning from thunderstorms may also cause brief rises in ozone, but lightning by itself is considered an insignificant contributor to the total ozone levels observed in rural areas (16).

The natural organic compounds emitted by vegetation may react to form additional ozone, or they may sometimes decrease it by scavenging reactions. The ozone added by reactions of natural hydrocarbons may increase the ambient ozone by 40 to 100 μg/m³ (0.02 to 0.05 ppm) (16). However, the atmospheric conditions that are conducive to higher ozone production by the photochemical process are not usually the same conditions associated with transport from the stratosphere. Therefore, the high values of nonurban ozone that are frequently above the standard cannot be attributed only to natural sources, but rather they appear to be primarily of man-made origin. The evidence for this conclusion is presented in the following section.

ATMOSPHERIC PHENOMENA THAT AFFECT OXIDANT CONCENTRATION

Recent measurements downwind of urban centers [Houston (17), Phoenix (17), Ohio cities (7), and Philadelphia (10)] demonstrate that transport of oxidants from urban centers to locations as far as 50 to 80 km (30 to 50 miles) downwind takes place. In Los Angeles, where the magnitude of oxidant generation is greater, the distance can be extended to 120 km (75 miles) or more downwind (18). Beyond these distances, it is difficult to distinguish the individual urban contribution of ozone from general nonurban levels. Therefore, although transport of oxidants may partially explain the high oxidant levels at short range downwind of urban centers, it has not been definitely shown that transport is the principal cause of the high readings at more remote sites. [A recent study by Bell Laboratories presented convincing evidence, from a statistical and episodic analysis, that ozone resulting from emissions from the New York City metropolitan area is transported by prevailing winds on a 300-km (187-mile) northeast trajectory through Connecticut and as far as northeastern Massachusetts (11).]

To date, the most positive method for demonstrating that the high ozone concentrations observed at more remote locations are at least partially due to emissions from man-made sources is by simultaneous measurements of ozone and compounds that are only emitted by human activity. Freon 11 is such a compound since it has no natural sources, is very stable in the lower atmosphere, and has a measurable but slowly increasing global background concentration of approximately 90 parts per trillion. An increase above this background concentration is strong evidence for transport of air from areas of human activity. In studies during 1973 and 1974 at Whiteface Mountain, New York, at Elkton, Missouri, and in the Pacific Ocean between Seattle and San Diego, no levels of ozone above 160 μg/m³ (0.08 ppm) have been found in which Freon 11 levels were not also above the background. Figure 2 shows ozone and Freon 11 measurements at Whiteface Mountain from July 24 to 27, 1974 (18). On July 24, ozone moved into the study area at 3 to 4 a.m. accompanied by an elevated Freon 11 level. July 25 was heavily overcast, and there was little ozone formation. July 26 was sunny; Freon 11 was at normal background concentrations, and ozone production was 100 μg/m³ (0.05

Table 1. Ozone levels above NAAQS at rural and urban stations from June 14 to August 31, 1974.

Station	Maximum Hourly Average Concentration (µg/m³)	Ninety-ninth Percentile (µg/m³)	Days Exceeding Standard* (percent)	Hours Above Standard	
				Number	Percent
Rural					
Wilmington, Ohio	370	260	58	259	14.9
McConnelsville, Ohio	330	240	56	239	13.3
Wooster, Ohio	330	260	55	262	14.0
McHenry, Maryland	330	270	43	262	13.0
DuBois, Pennsylvania	400	310	54	341	20.5
Urban					
Canton, Ohio	280	230	44	148	8.0
Cincinnati, Ohio	360	220	20	54	3.5
Cleveland, Ohio	270	200	26	51	3.0
Columbus, Ohio	340	220	27	113	5.8
Dayton, Ohio	260	220	35	114	7.2
Pittsburgh, Pennsylvania	300	230	37	106	6.5

Note: 1 µg/m³ = 0.0005 ppm.

*Based on data available from each station.

Figure 1. Location of ozone ground sampling stations in 1974 study.

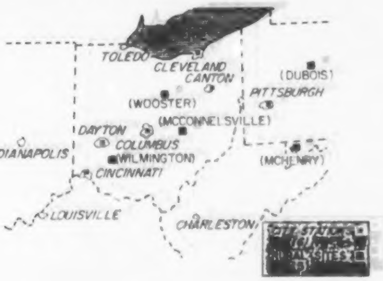
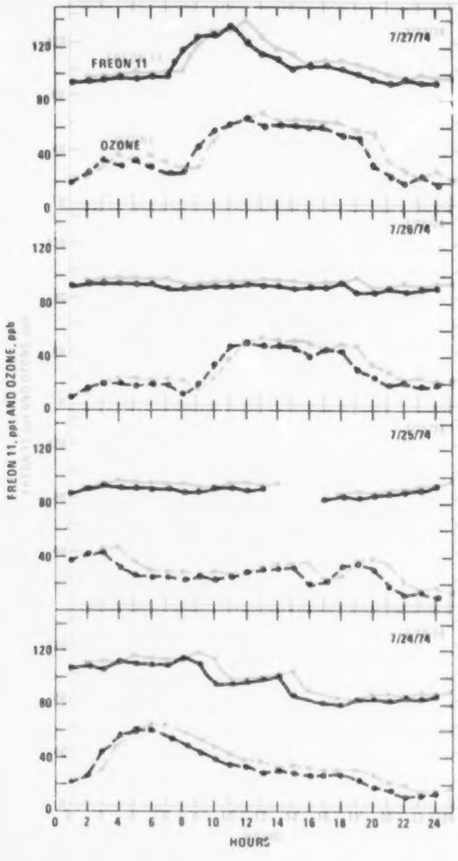

TOLEDO
CLEVELAND
CANTON
(DUBOIS)
(WOOSTER)
PITTSBURGH
(MCCONNELSVILLE)
DAYTON
COLUMBUS
INDIANAPOLIS
(WILMINGTON)
(MCHENRY)
CINCINNATI
LOUISVILLE
CHARLESTON

Figure 2. Hourly averages of Freon 11 and ozone at Whiteface, New York.



ppm) during the day. On July 27, there were elevated Freon 11 concentrations, so that the ozone concentrations may have been due to local production and to ozone or precursors transported to the area. Thus, the higher levels of ozone measured on July 24 and July 27 are associated with high Freon 11 levels, which implies that these pockets of air had been transported from some area where man-made emission sources are present. Similar studies were performed by investigators in England (20). They concluded that a significant portion of the ground-level ozone in southern England is caused by transport of precursors or ozone over distances of the order of 100 to 1000 km (160 to 1,600 miles).

Air parcel movement in the eastern United States was related to ozone concentration by Bach (21) using a trajectory computer program developed by the EPA Meteorology Laboratory. These trajectories computed air parcels arriving at the various nonurban ozone measuring sites in the summer of 1973. Sets of trajectories for 2 sites for the upper and lower decile of 12-hour average ozone concentrations are shown in Figures 3 and 4. The trajectories are for the 90-kPa (900-millibar) level [approximately 900 m (3,000 ft) above sea level], corresponding roughly to the mean afternoon mixing height.

Past positions at 12, 24, and 36 hours are plotted for 12-hour average ozone concentration periods falling in the upper and lower 10 deciles. The trajectories are inconclusive, showing no definitive pathway pattern differences between high and low ozone periods. It was significant, however, that for high ozone periods past positions are more closely spaced than for low ozone periods, indicating generally slower air movement. It is postulated that, for high rural ozone occurrence, light wind flow likely associated with longer reaction periods, slow-moving highs, and accumulation of ozone are of greater importance than the particular trajectories followed during long-range transport.

Temperature

It has generally been noted in the monitoring of ozone at various locations in this country that ozone concentrations above the NAAQS level occur during the warmer months of April through October. Seldom are such levels found to occur at other times of the year, except during warmer periods, mostly in the southern tier of states. Smog chamber experiments by Jeffries show that, at daily maximum temperatures below about 14.5 C (58 F), significant generation of ozone does not occur. For the 1973 field study data, Bach (21) correlated maximum hourly ozone concentrations for each day at each of the 4 sites with the maximum daily temperature at nearby surface stations of the National Weather Service. The paired stations were as follows:

Ozone Station	Temperature Station
McHenry, Maryland	Elkins, West Virginia
Kane, Pennsylvania	Youngstown, Ohio
Coshocton, Ohio	Columbus, Ohio
Lewisburg, West Virginia	Beckley, West Virginia

The results for 2 sites are shown in Figure 5. A consistent statistical relation was found with increase of maximum hourly ozone concentration related to increasing maximum temperature. The best correlation found was 0.71 for the McHenry-Elkins pair. In no case was an ozone concentration of greater than 160 $\mu g/m^3$ (0.08 ppm) found with temperatures less than 16.5 C (61.5 F).

The trend for higher ozone concentrations with greater maximum temperatures does not necessarily establish that a direct relation exists. Maximum temperature is also a function of other meteorological variables, including sky cover, synoptic weather features, wind speed, and past history of the air mass. However, direct or indirect,

Figure 3. Trajectories associated with high and low decile, 12-hour average ozone concentrations at McHenry, Maryland (squares and triangles indicate 12-hour past positions prior to arrival at indicated stations).

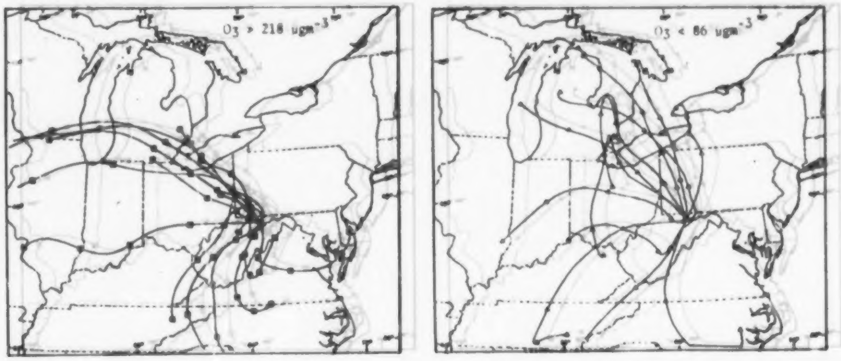


Figure 4. Trajectories associated with high and low decile, 12-hour average ozone concentrations at Coshocton, Ohio (squares and triangles indicate 12-hour past positions prior to arrival at indicated stations).

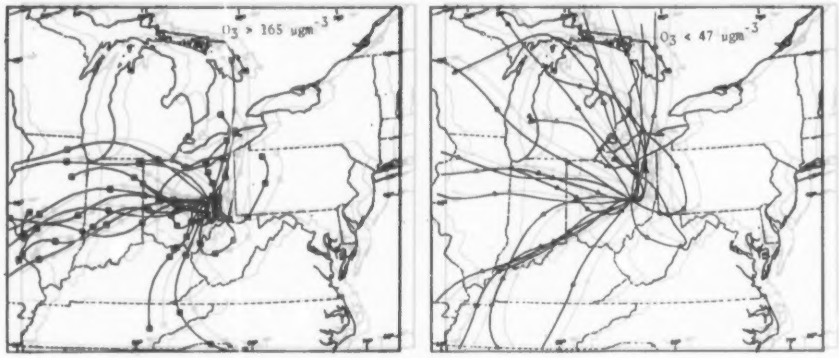


Figure 5. Scatter diagrams and least squares fit of daily maximum hourly ozone concentration and maximum daily temperature at indicated stations (A indicates 1 occurrence, and B indicates 2).

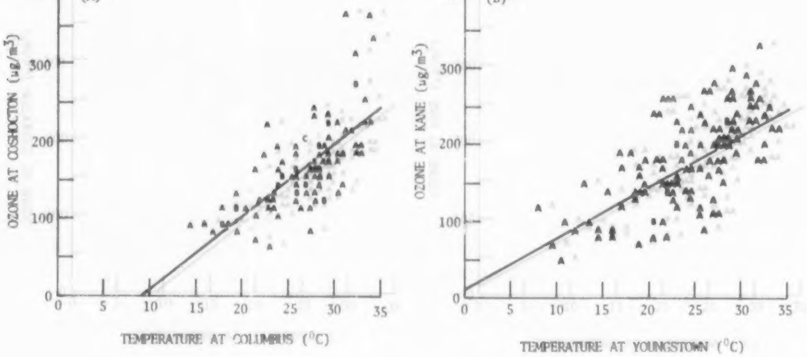


Figure 6. Time sequence of 12-hour average ozone concentrations at McHenry, Maryland, in 1972 (8 a.m. to 7 p.m. EDT is unshaded, 7 p.m. to 8 a.m. is shaded, and frontal passages are shown by double arrow).

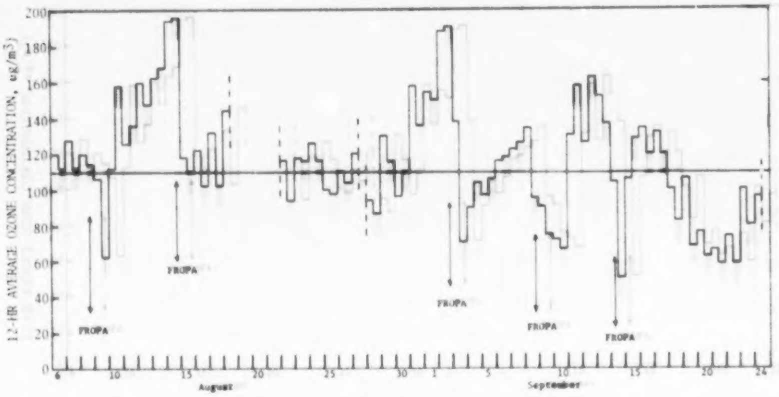
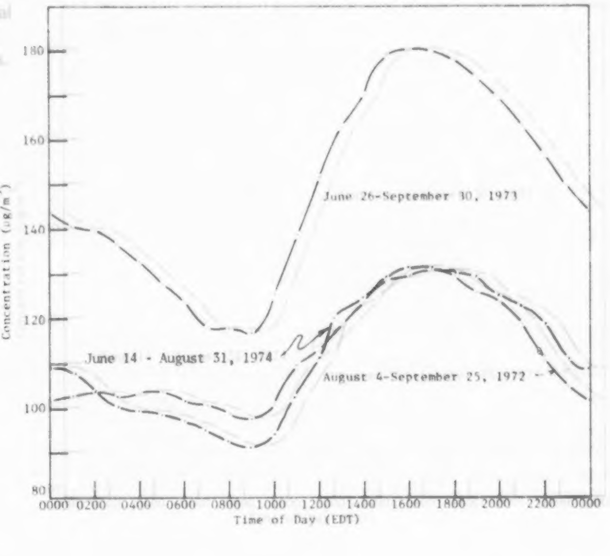


Figure 7. Comparison of mean diurnal ozone concentration at McHenry, Maryland, for indicated study periods.



maximum temperature appears to be a reliable indicator of the potential for high ozone concentrations to occur.

Fronts

In the analysis of the 1972 ozone measurements, a definite pattern seemed to be present of buildup of concentration levels followed by sharp decreases following frontal passages. This pattern is shown in Figure 6. This pattern is consistent with what is generally experienced with other pollutants, especially those in urban areas. A similar analysis was performed on the 1973 ozone data, but curiously the pattern exhibited the previous year did not seem to repeat itself very often. A possible reason for the lack of repeatability was the fact that frontal movements recorded in 1973 were almost all classified as weak. Therefore, they may have lacked the vigorous vertical mixing and flushing action normally experienced during frontal passages. This may help explain the data shown in Figure 7, in which generally higher ozone levels were experienced in 1973 relative to 1972 and 1974 at the rural site near McHenry, Maryland.

Vertical Distribution of Ozone

The data shown in Figure 7 indicate the diurnal variation in the average hourly concentrations. This pattern has been relatively consistent during the 1972 to 1974 studies. Generally, the highest ozone concentrations occur in the late afternoon and the lowest occur in the early morning. In general, there is no significant variation among monitoring locations, although the pattern is more pronounced at those rural locations that are subject to periodically strong inversion formation.

Figure 8 shows vertical ozone profiles that were taken 3 times during 1 day during the 1974 summer studies (7) and that illustrate the effect that low-level atmospheric stability has on ozone concentrations. These profiles are similar to other vertical measurements at Indianapolis and Canton, Ohio, and are consistent with ozone soundings of previous years. The concentrations of ozone decrease above the subsidence inversion near 2400 m (8,000 ft) as shown by the temperature profiles. The early morning profile indicates low ozone concentrations (40 $\mu g/m^3$ or 0.02 ppm) beneath a radiation inversion that occurred between the surface and 600 m (2,000 ft). Trapped between these 2 inversions is a layer of ozone above 180 $\mu g/m^3$ (0.09 ppm) that had formed on previous days and had persisted through the night. In this layer, ozone has been separated from ground-based scavenger pollutants and may persist for long periods of time and may be transported over long distances. At the surface below the radiation inversion, ground emissions of natural destructive agents and surface features provide a sink for the ozone. During the day, as the low-level radiation inversion layer dissipates, the lower atmosphere becomes well mixed, and oxidant, formed by photochemistry from precursors emitted at the surface or from hydrocarbons left over from the previous day, mixes with the layer of ozone that had persisted through the night. As the day progresses, more oxidant is formed as shown by the high oxidant concentrations measured in the afternoon.

This typical pattern explains the usual diurnal oxidant concentrations measured at ground-based rural monitors. This pattern usually shows concentrations that are low at night and that build up and become high in the afternoon. Exceptions occur when high oxidant concentrations have been measured at night under atmospheric conditions that dissipate or prevent formation of the surface-based inversion. Also, during prolonged stagnation episodes, ozone concentrations build up without appreciable decrease in ozone levels at night. It is hypothesized that strong surface-based inversions fail to materialize at night during hazy or smoggy conditions so that vertical exchange within the lowest tropospheric layers may be sufficient to maintain high surface ozone concentrations.

Pressure Systems and Surface Winds

For some episodes of high ozone, studies have shown (8, 9) that similar ozone concentrations were measured at widely separated rural sites. During these episodes urban areas were also observed to experience high concentrations of ozone.

Analysis of data from the Research Triangle Institute summer studies indicates that ozone concentration variation is associated with large-scale weather features related to high-pressure weather systems (7). Figure 9 shows a smoothed graph of surface pressure and surface ozone concentrations for 1973 averaged over several eastern study sites. The highest oxidant readings occurred during periods of high pressure; however, as explained below, high pressure in itself does not lead to high ozone.

Figure 8. Ozone profile flight at Wilmington, Ohio, August 1, 1974.

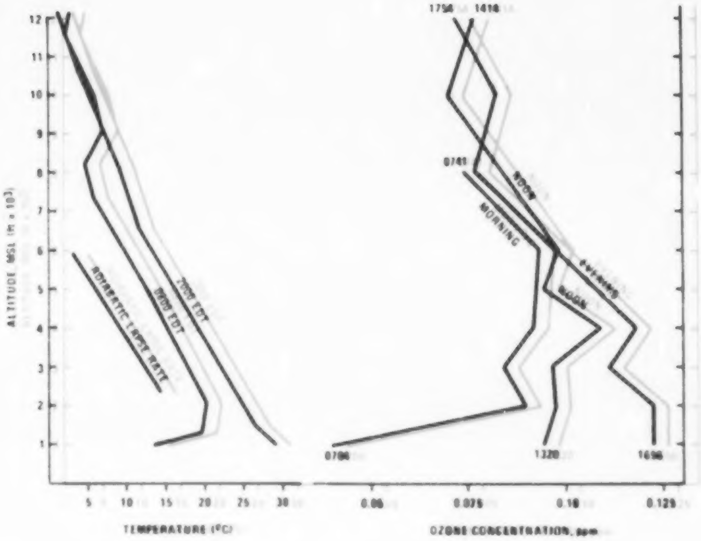


Figure 9. Smoothed variations for area average daily ozone and surface pressure (1973 time sequence).

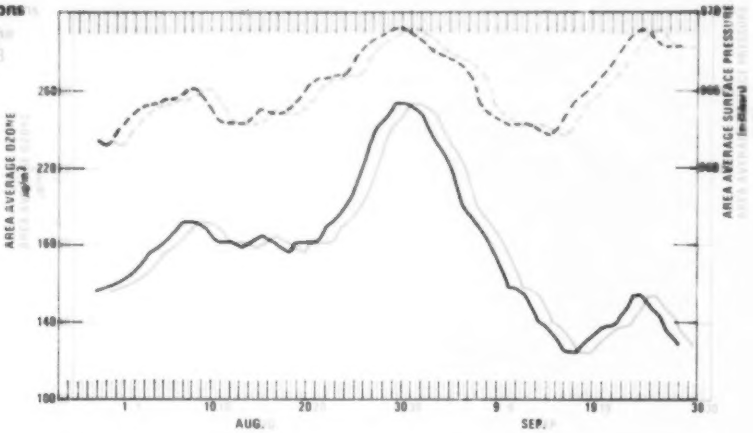
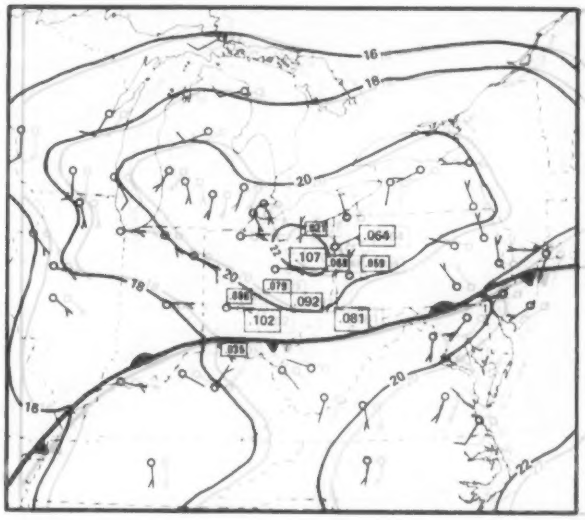


Figure 10. Average ozone concentration, July 6, 1974.


16
18
20
.064
.107
.092
.102
.081
.079
.086
.068
.069
.035
18
20
16
22

On a spatial basis, the higher ozone concentrations generally seem to occur near the central portion of high-pressure cells and decrease outward. The spatial distribution of ozone in a high-pressure system is shown on weather maps for July 6 and July 8, 1974, in Figure 10 and Figure 11 (7). These are 2 of several cases studied. The 5 numbers in large boxes are the 8-hour afternoon averages of ozone concentrations in parts per million observed at the rural monitoring sites. The 6 numbers in smaller boxes are the ozone concentrations at urban locations. The contour lines are lines of constant pressure. The center of the high-pressure system is over Cleveland on July 6 (Figure 10) and is indicated by the line numbered 22 (102.2 kPa or 1,022 millibars). On July 8 (Figure 11) the high-pressure cell is centered over western Pennsylvania. The wind direction and velocity is shown by the arrows. The shading indicates areas of high man-made hydrocarbon emissions where emission densities are greater than 3500 kg/km^2/year (10 tons/mile^2/year). In the urban areas emission densities are between 35 000 and 350 000 kg/km^2/year (100 and 1,000 tons/mile^2/year). Emission densities are high in most of this region and are sufficient to account for the measured ozone concentrations. The evidence suggests that near the center of a high-pressure area, perhaps 160 to 320 km (100 to 200 miles) in diameter, environmental conditions are most conducive to high oxidant buildup. Apparently, near the center of the high-pressure area, there are light disorganized winds, sufficient ultraviolet radiation, and high temperatures; and if sufficiently large emissions of precursor compounds are present, oxidants will be formed. Thus, in a slow-moving high, a virtual outdoor smog chamber develops in which locally generated oxidants are added to oxidants and precursors that may have been transported into the area as the high-pressure cell was developing.

The summer studies by Rasmussen (17) in the Canton, Ohio, area also related high concentrations of ozone to slowly moving high-pressure systems. He found that Canton frequently experienced advection of oxidant from contamination sources that became a part of the anticyclonic (high-pressure) air mass. The model developed by Rasmussen (17) is shown in Figure 12. Behind the central portion of the high-pressure system, the high concentrations appeared late in the day or early in the morning, when photochemical reactions from local pollutants would not be occurring.

Whether the highest concentrations of ozone occur in the center or on the trailing edge of the high-pressure system will depend on the source of emissions and the specific movement of the system. The conclusion of the above studies is that migratory anticyclones achieve a widespread level of ozone in the air mass and that the urban areas with high precursor emissions are the predominant sources of the high rural ozone concentrations.

ASSESSMENT OF RURAL OZONE STUDIES

The recent laboratory and field investigations of oxidant formation have provided several new insights or strengthened past understanding. It is now apparent that oxidants are a rural as well as an urban problem. Oxidants can be formed during long time periods of stagnant conditions in high-pressure systems or during transport of oxidants and precursors. This implies that the long-term behavior of oxidants and precursors is an important contributor to oxidant concentrations. Figure 13 shows a qualitative model of the components of the origins of ozone measured in the rural to urban to rural movement of ozone (15). This model indicates the man-made, stratospheric, and natural hydrocarbon sources of ozone upwind of a city. It indicates the scavenging effect of the emissions in the urban area and the buildup of an ozone plume downwind of the urban center. It is the conclusion of the recent studies that, although natural sources of oxidants may at times contribute to ozone concentrations reaching levels near the oxidant standard, man-made emissions are the predominant source of the highest levels of ozone. The occurrence of high levels of ozone in rural areas also indicates that additional control measures may be required in order to achieve the oxidant standard nationwide (22).

Figure 11. Average ozone concentration, July 8, 1974.

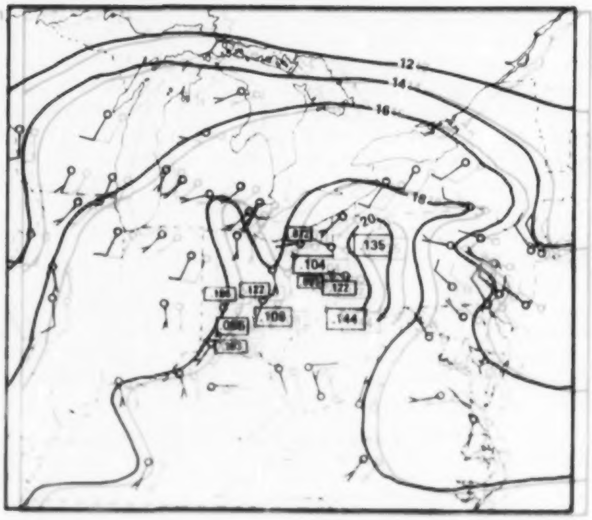

12
14
16
18
20
.135
.104
.122
.108
.144
.122
.086

Figure 12. Ozone behavior within a high-pressure air mass.

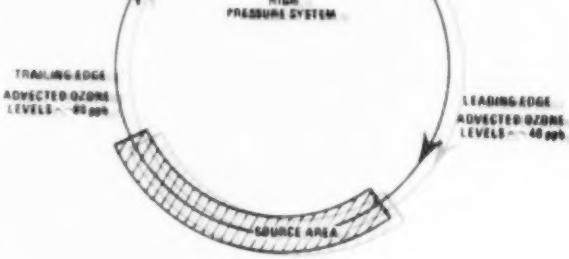
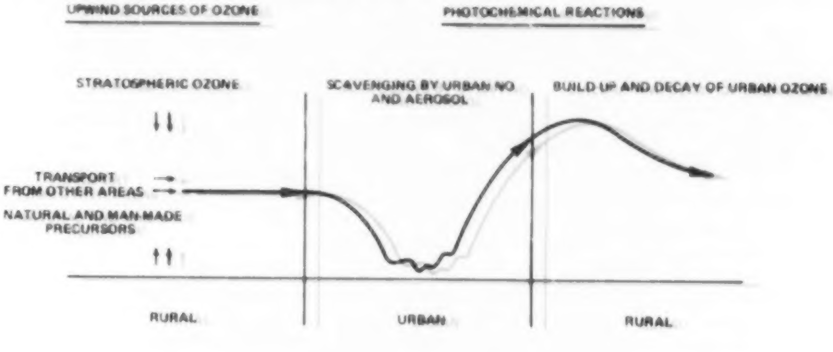

HIGH
PRESSURE SYSTEM
TRAILING EDGE
ADVECTED OZONE
LEVELS ~ 80 ppb
LEADING EDGE
ADVECTED OZONE
LEVELS ~ 40 ppb
SOURCE AREA

Figure 13. Surface ozone formation and transport.


UPWIND SOURCES OF OZONE
PHOTOCHEMICAL REACTIONS
STRATOSPHERIC OZONE
SCAVENGING BY URBAN NO AND AEROSOL
BUILD UP AND DECAY OF URBAN OZONE
TRANSPORT FROM OTHER AREAS
NATURAL AND MAN-MADE PRECURSORS
RURAL
URBAN
RURAL

SUMMARY

The information presented in this paper is based on recent field-monitoring programs for ozone in nonurban areas. The paper presents a discussion of the factors that may lead to and affect the observed ozone concentrations. Several meteorological parameters including transport of ozone and its precursor compounds are examined as factors affecting rural ozone levels that exceed the national ambient air quality standard. The conclusion is that man-made sources of precursor compounds are primarily responsible for the violations of the air quality standards. Transport of ozone or ozone precursors from cities into nonurban areas and the importance of synoptic-scale pressure systems are discussed.

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EXAMINATION OF REGIONAL PHOTOCHEMICAL MODELS BY A USER

Andrew J. Ranzieri and Earl C. Shirely, Division of Construction and Research Transportation Laboratory, California Department of Transportation

During 1974 and 1975, there was considerable discussion of the use of regional photochemical models to assess the impact of transportation systems on the air environment. Considerable progress was made to provide operational computer models that can be used by transportation planners and engineers. However, certain issues involving data input requirements and model refinements must be resolved before transportation planners are able to apply photochemical models for planning activities. The purpose of this paper is to discuss, from the user's point of view, the broad application of photochemical modeling, input data requirements, appropriateness of existing data sources, possible solutions to updating air quality data bases, and modeling approaches that are available to solve practical transportation planning problems.

APPLICATIONS OF REGIONAL PHOTOCHEMICAL MODEL FOR TRANSPORTATION PLANNERS AND ENGINEERS

We all recognize that an air model is an essential component of planning studies because of the need to establish a quantitative relation between emissions and their resulting ground-level pollutant concentrations. Every urban area has unique climatological and meteorological conditions. The spatial distribution of emissions, as well as the composition of these emissions, varies from city to city. The concentrations of secondary pollutants, formed in the atmosphere through the chemical reactions of primary (emitted) pollutants, are influenced by local meteorology, emissions patterns, intensity of solar radiation, and many other variables. Clearly, to predict the spatial and temporal distributions of ground-level concentrations of air pollutants requires that account be taken of these many complexities through the simulation of physical and chemical processes that actually give rise to the air quality observed.

A photochemical model can be defined as a mathematical representation of air movements and chemical reaction processes that, when combined with emissions and meteorological data, can be used to predict the temporal and spatial distribution of air pollutants. Air quality models can be used as a "tool" in the decision-making process provided the models have been verified with actual field measurements and quality input data are available. Under these conditions, models can assist transportation planners and engineers to

1. Assess the impact of highways or multimodal transportation systems on air quality;
2. Provide a systematic procedure to evaluate the interrelations of land use, transportation, and air quality;
3. Select the locations for future transportation facilities to minimize the air quality impacts (spatial alternative);
4. Evaluate the impact of transportation control plans;
5. Estimate air quality for areas in which pollutant measurements are unavailable; and

6. Comply with federal and state legislation concerning environmental impact assessment.

MODELING APPROACHES

Air quality models are generally based on the solution of the conservation-of-mass equation. The conservation-of-mass equation for a given air pollutant species and chemical reactions can be expressed as

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x}\left[K_H\frac{\partial c_i}{\partial x}\right] + \frac{\partial}{\partial v}\left[K_H\frac{\partial c_i}{\partial y}\right] + \frac{\partial}{\partial z}\left[K_z\frac{\partial c_i}{\partial z}\right] + R_i + S_i \qquad (1)$$

where

c_i = concentration of pollutant species i;
x,y,z = Cartesian coordinates;
u,v,w = wind speed in the x, y, and z directions respectively;
K_H,K_z = horizontal and vertical turbulent diffusivities;
R_i = rate of production of species i through chemical reactions; and
S_i = rate of production of species i from source emissions.

The numerical solution of equation 1 (1) is solved by using either a Eulerian or a Lagrangian coordinate system. The Eulerian coordinate system is fixed to the surface of the earth, and the Lagrangian coordinate system is a moving system. The Eulerian solution is commonly referred to as a grid model, and the Lagrangian solution is referred to as a trajectory model.

In the grid model the study region is divided into a 3-dimensional array of cells (Figure 1). Each cell can vary from 1 to 4 km (0.6 to 2.5 miles) on a side and on the order of 10 to 100 m (33 to 330 ft) high. The size of each cell, of course, will depend on the size of the study area, spatial distributions of emission fluxes of pollutants, terrain affects that may alter the surface winds, and inversions. The solution of equation 1 is achieved by numerically integrating the equation in 3-dimensional space and in time over each grid.

In the trajectory model, a column of air is followed through the study area as it is moved by the surface winds. The air pollutants are emitted into the column as fluxes at the ground surface. As the column passes over the study area, chemical reactions take place within the column.

Existing regional air quality models are capable of predicting the temporal and spatial distribution of concentrations for the following pollutants: carbon monoxide (CO), nitric oxide (NO), nitrogen dioxide (NO_2), ozone (O_3), unreactive hydrocarbons (URH), and reactive hydrocarbons (RHC). The unreactive hydrocarbons are generally taken to be methane, propane, benzene, and acetylene.

Clearly, for each grid square, a description of the temporal and spatial distribution of emissions (both stationary and mobile), meteorological conditions, and initial air quality concentrations must be specified, or calculated from known data. (Only for the initial first hour of simulation must the concentration fields be known or calculated.)

INPUT TO REGIONAL PHOTOCHEMICAL MODELS

A common trait of all regional photochemical models is their need for vast amounts of emissions, meteorological, and air quality data. The greater the quality of the data base is, the better is the ability of the model to simulate events in the atmosphere with

Figure 1. Typical grid study area for Los Angeles.

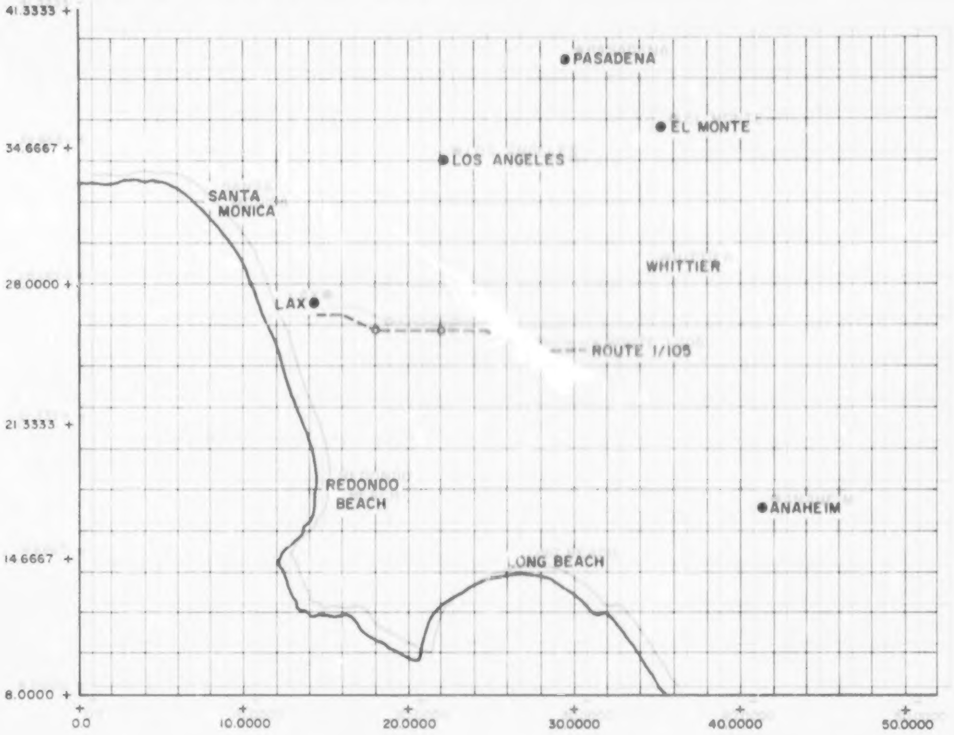
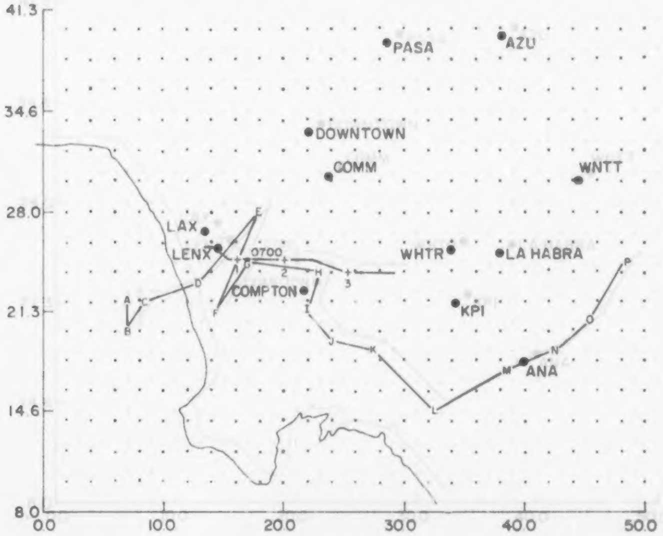

PASADENA
EL MONTE
LOS ANGELES
SANTA MONICA
WHITTIER
LAX
ROUTE 1/105
REDONDO BEACH
ANAHEIM
LONG BEACH
41.3333
34.6667
28.0000
21.3333
14.6667
8.0000
0.0
10.0000
20.0000
30.0000
40.0000
50.0000

Figure 2. Typical trajectory simulation for Los Angeles area.


PASA
AZU
DOWNTOWN
COMM
WNTT
LAX
LENX
0700
WHTR
LA HABRA
COMPTON
KPI
ANA
A
B
C
D
E
F
G
H
I
J
K
L
M
N
O
P
1
2
3
41.3
34.6
28.0
21.3
14.6
8.0
0.0
10.0
20.0
30.0
40.0
50.0

a higher degree of confidence. First, the emission inventories (both mobile and stationary sources), meteorology, and the initial hour of air quality data throughout the region are needed so that the model can simulate the transport and diffusion of the emission fluxes while it attempts to duplicate the chemical reactions that occur in the atmosphere. Second, air quality data are required so that air quality predictions can be compared with real-world observations. This verification allows confidence in the model so that it can be used for predicting future pollutant concentrations for air quality impact assessment.

Emission Inventory

The emission inventory must provide estimates, by category, of vehicular, aircraft, power plant, refinery, and distributed area sources including their temporal variations. The emission sources spatially distributed over a grid system (Figure 1) must have a temporal resolution of 1 hour because the air quality standards are generally based on a 1-hour exposure time. For the emission inventory, the following information is required (2). For all of the emission inventories, the ratio of NO to NO_2 is also needed.

Vehicles

Information required for vehicles is

1. Spatial distribution of daily vehicle kilometers traveled (vehicle miles traveled, VMT);
2. Temporal (hourly) distribution of vehicle kilometers traveled;
3. Average emission rates (mass/distance) of CO, NO_x, and HC;
4. Spatial and temporal distributions of average vehicle speed;
5. Variations in emission rates with average speed for CO, NO_x, and HC; and
6. Effects on average emissions rate of cold-start and hot-running operations.

Aircraft

Information required for aircraft is

1. Ground operations emission rates of CO, NO_x, and HC as a function of traffic level, mode of operation, aircraft class or type, location, and time; and
2. Flight operation emission rates as a function of the same variables as those of ground operations emission rates, but segmented into taxi, landing, and takeoff modes.

Power Plants

Power plant information is

1. Emission rates of NO_x for each plant as a function of type of fuel burned, time of day, and time of year;
2. Emission rates of NO_x and organic gases for each refinery; and
3. Emission rates of CO, NO_x, and organic gases for distributed stationary sources as a function of location.

Meteorological Data

The meteorological data, treated entirely as input to the model, in the most comprehensive form include the items listed below:

1. Wind speed and direction, both at the surface and aloft, as a function of location and time;
2. Temperature as a function of height (to permit estimation of stability), location of the inversion layer and inversion base, and strength of the inversion;
3. Vertical turbulent diffusivity as a function of height, ground location, and time of day (this is estimated from various correlations as a function of turbulent energy dissipation rate, wind shear, vertical temperature gradient, wind speed, and surface roughness); and
4. Insolation as a function of ground locations, elevation, and time of day.

Initial Concentration Fields

The air quality data required to establish initial concentration fields at the surface and aloft for a full 3-dimension simulation are concentrations for CO, NO, NO_2, O_3, RHC, and URH. The richness of such a data base described in the above varies within a given region based on the availability of obtaining a complete and up-to-date emission inventory, number of surface air and meteorological monitoring stations and their separation distance, and the frequency of measurements of vertical temperature profiles and wind and air quality data aloft.

PROBLEMS WITH USING EXISTING AIR QUALITY DATA BASES

Many urban areas appear at first glance to have a sufficient emission inventory and an aerometric data base that can be used in photochemical models. This observation is generally based on the number of air monitoring and meteorological stations that exist in a given network. Before making a hasty decision that the inventory is adequate, however, one should be able to answer the following questions.

1. Are the air and meteorological monitoring stations located such that they measure representative data consistent with model assumptions to describe the temporal and spatial distribution of surface winds and air quality?
2. Are the air monitoring networks located near a localized source of pollutant emissions?
3. Is there a standardized height above the ground surface for the entire network from which the air and meteorological measurements are made?
4. Are the recorded hourly values of air quality concentrations and surface wind measurements based on an integrated hourly average or instantaneous reading?
5. How often are the air and meteorological instruments calibrated to provide quality assurance control of the data collected?
6. Are stationary source inventories up to date?
7. Is the vehicular emission inventory based on the latest emission factors published by U.S. Environmental Protection Agency?
8. For the year in question, do transportation simulation models used to estimate vehicle kilometers traveled consider that the price of gasoline has doubled? What effect, if any, has this had on the estimates of vehicle kilometers traveled for the region?

These are just some of the more obvious questions that transportation planners and engineers should consider before using any existing data. If, for the existing data base, satisfactory answers to the questions cannot be evaluated, then the user is confronted with the decision of providing an initial investment to obtain quality inputs. A discussion of the problems is described below.

Definition of Grid Boundaries or Study Region

The first step involved in applying a regional air quality model is to decide on the size of the study area. Because of the multidisciplinary expertise required to develop inputs for the models, the exact boundaries for an urban area should be coordinated with local land use planning agencies, air pollution control districts, and transportation planners. Major factors to consider in defining the region should include populated areas, areas of high pollutant concentrations, areas of high emissions, topography and terrain features, and local master plans for future developments. All agencies involved must agree to a common region, coordinate system, and origin of study area. The grid size is selected next. The surface grid sizes commonly used at present are 2×2, 3.2×3.2, and 5×5 km (1.2×1.2, 2×2, and 3.1×3.1 miles). However, the size of each grid will determine the size of the entire study area. At present, the maximum number of grids allowed in regional models varies from 25×25 to 50×100. Therefore, if a grid size of 3.2×3.2 km (2×2 miles) on a side is selected and the model has a maximum of 25×25 grids, then the study area will cover an area of 80×80 square kilometers (50×50 square miles).

In some cases, to expand the grid size requires changes in the computer program. Therefore, care must be taken not to exceed the maximum number of grids. Once the origin and grid size have been selected, then all the emissions for mobile and stationary sources must be located based on this coordinate system and grid. In general, the emission inventory for mobile and stationary sources is developed by different agencies. In California, for example, vehicular emissions are developed by the California Department of Transportation, and stationary emissions are developed by local air pollution control districts or the California Air Resources Board (ARB). Each agency has a different coordinate system to geocode emission sources. This can create problems for the user in acquiring data for each grid square and allocating the proper emissions from both mobile and stationary sources.

Emission Inventory

Emission input into a regional model is generally developed by separate agencies. Problems that arise in obtaining emissions are numerated below.

1. It is difficult to obtain vehicle kilometers traveled allocated to each grid square calculated from transportation models.
2. Transportation simulation models used to predict vehicle kilometers traveled are insensitive to changes in gasoline prices, and that may affect predictions of vehicle kilometers traveled.
3. No recent verification studies have been made of transportation simulation models to evaluate their predictive capabilities based on current travel behavior.
4. In predictions of future vehicle kilometers, the present transportation simulation models cannot respond to changes in highway assignments when gasoline prices are doubled or transit alternatives are considered.
5. Growth rates in present transportation models may not be representative of future trends in population growth within the local community.
6. The ability of transportation models to predict speed on links without some hand adjusting is doubtful.
7. The representativeness of the highway cruise-mode emission factors as published by EPA is questionable.
8. The aircraft emission data are not available as required by air quality models.
9. Stationary source inventories are not up to date and are generally 2 to 3 years behind.
10. Future stationary source inventories from local and state agencies are difficult to obtain.
11. Different air pollution agencies have no consistency in defining reactive hydrocarbons, and this makes it almost impossible to use second-generation kinetic mechanisms that group hydrocarbons into 5 classes of methane, paraffins, olefins, aromatics, and aldehydes.

Existing Meteorological Data Bases

The existing sources of meteorological data for use in regional models are primarily airports and air pollution control district air monitoring stations. The meteorological data monitored consist of surface wind speeds and directions, and in some instances, information from 2 daily radiosonde releases to obtain the vertical temperature profile data. Before examining the existing data, one must keep in mind that the meteorological data will be used to calculate the representative 1-hour wind flow fields on a temporal and spatial basis for the entire study area for each grid. The same applies to the temperature measurements that the existing data must be able to represent and describe the temporal and spatial changes of inversions for the entire area. The following problems arise when existing data are used.

1. In most areas, there are too few ground stations to describe the surface wind flow field.
2. In many cases the instruments tc monitor surface winds are insensitive to low speeds less than about 1.35 m/s (3 mph).
3. The readings recorded at airports are generally instantaneous and are not generally representative of the 1-hour average.
4. The air pollution control district wind stations are generally located on tops of buildings and monitor the localized air flow around and over the building and not the representative surface winds.
5. In regions where terrain effects alter the inversion by thermal heating, 1 or 2 radiosonde releases are not representative for the region, nor are they sufficient to describe the temporal behavior.
6. Virtually no measurements are made of winds aloft.
7. Virtually no measurements of insolation are made. If they are, it is generally at only 1 location. This makes it difficult to account for spatial variation in radiation intensity in large urban areas.

Existing Air Quality Data Base

Most of the existing ground air monitoring stations operated by state and local air pollution control districts are located at sites (a) where real estate is inexpensive and (b) where stations are not a great distance apart so that instrumentation technicians can service and check the daily operations. These stations are not located or intended to be used to provide input to a data base or verify regional air quality models. The following problems exist with existing air quality data.

1. The number of ground stations is insufficient to describe the temporal and spatial distribution of pollutants for establishing the initial concentration fields for model inputs or to provide a satisfactory data base to verify models.
2. There are no standards for exposing the air intake or locating the stations. Most stations are located near major surface streets and monitor the local exhaust emissions from vehicles. To confuse the situation further, there is no standard height that the air intake must be above the ground surface. Based on our experiences, the height of the air intake can vary from a 1- to an 8-story building. With this kind of exposure (low air intake and near surface streets), the air monitoring stations generally monitor high concentrations of CO, HC, and NO_x because of nearness of the source. However, reduced values of O_3 may be monitored because of the reaction of NO (emitted from motor vehicles) and ambient O_3 resulting in higher NO_2 concentrations and a depletion of O_3. The reverse may be true when air intake is located on a tall building, i.e., low CO, HC, and NO_x concentration and high O_3. Therefore, the representativeness of these stations is questionable for use as regional modeling input and verification.
3. Air quality measurements aloft are virtually lacking in urban areas. This information is important in determining the initial concentration fields in the models and is also required to treat the O_3 buildup beneath the elevated inversion that can vary from

day to day.

4. Air quality instrumentation used is not comparable from one location to another. Wet chemical methods are used in some urban regions, and dry chemical techniques or a combination of both is used in others. This does not provide continuity in measurements unless careful correlation of instruments is made.

5. A frequent program of calibrating the instruments used in air monitoring stations is lacking. This is necessary to ensure quality data for model applications. Based on our experiences, the frequency of calibration varies from 6 months to 3 years. More typically, it is 1 year or more.

6. The ability of all stations within a network to monitor reactive and total hydrocarbons (RHC and THC) is lacking. In some urban areas only selective stations monitor RHC and THC, and almost all monitor THC. A few partial stations monitor for O_3 only.

Verification of Photochemical Models

Confidence in using regional photochemical models can only be achieved when model predictions are compared to real-world measurements. At present, with the exception of EPA's St. Louis study, not a great deal of attention has been given to monitoring programs to provide measurements of air and meteorological data at the surface and aloft that can be used as inputs to verify regional photochemical models. This should be obvious from the previous discussions. In many instances, reviewing agencies, such as EPA, require that, before a model is used for decision making, the predictions made by the model be compared to actual field measurements and the performance of the model be evaluated accordingly.

Customizing Regional Models for Urban Areas

To our knowledge, all of the existing photochemical models (1, 3, 4) were developed for the Los Angeles basin under contract to EPA. The models developed were, therefore, more of research tools designed specifically for the Los Angeles study area, which is 80×80 square kilometers (50×50 square miles). The computer programs written were customized for the size of the region, the description of the temporal and spatial variation of inversions, and the mountain barriers that alter surface winds for the Los Angeles area. Therefore, to use the existing programs for other regions requires internal changes in the computer code. This is an additional cost to users whether they make the changes themselves or contract with the developers of the models.

Institutional Constraints

Because the models were designed specifically for the Los Angeles area, the models were not written in an efficient manner to be applied to other urban areas. For example, to take the grid model of Systems Applications, Inc. (SAI) and expand the original 25×25 grid system to 50×100 grids (which is required in the South Coast air basin in California) and run a 10-hour simulation on an IBM 370/168 computer system would cost about $2,000 a run. This would require about 16 hours residence time on a typical IBM 370/168 system and would mean, if it were practical, that runs would probably have to be made on weekends only. On a comparative basis, running the original 25×25 grid for 10 hours of simulation on the IBM 370/168 system would cost about $240 with a residence time of about 2 hours in the computer center. On the other hand, studies made by SAI have shown that, if the same programs were converted to a CDC 7600 computer system and run at the Lawrence Berkeley Laboratory, the cost would be reduced by about a seventh or $35 and $300 per 10-hour simulation run for the 25×25 and 50×50 grids respectively. This illustrates that, depending on the number of grids and the user's computing system, it may or may not be possible to use the SAI model on a practical basis.

If a trajectory model (3) is used for the 25×25 grid and run on the IBM 370/168 system, the cost for a 10-hour simulation run for 1 trajectory is about $20. A comparison of the cost of running a trajectory versus a grid model is misleading because to obtain results similar to the grid model output for a 25×25 grid would require hundreds of trajectory simulation runs. The advantages and disadvantages will be discussed in a later section.

There are some other general operational problems with the existing regional models. The regional models were developed by chemists, physicists, meteorologists, and engineers rather than by transportation planners or highway engineers. Difficulty arises in interfacing the vehicular emission output from transportation simulation models into the air quality model. The emissions depend on the number of links, type of trip, and temporal patterns. The model developers need to coordinate their efforts to provide a more workable package for users. Another problem that arises is that the user instruction manual written by the developers of the air quality models is not oriented for highway engineers but is more suitable for computer programmers. Therefore, the instruction manual needs to be rewritten so that air quality models can be more generally implemented. The computer programs also need to be rewritten to make them more efficient.

SOLUTIONS TO UPDATING AIR QUALITY DATA BASES FOR AIR QUALITY MODELS

The above discussion made it apparent that, in the user's view, the quality of input into regional air quality models has a high degree of uncertainty. In addition, there are computer operational problems. Input includes the emission inventories and the aerometric data bases. High quality of input variables used in the models can result in a more systematic and scientific evaluation of model performance. This conclusion assumes that the user has confidence in the concept of mathematical modeling and confidence in the ability to improve on the model predictions. One part of improving model inputs and predictions requires a field monitoring program to collect an aerometric data base. The design of this aerometric data base should be based on obtaining measurements that are spatial and not point oriented. This means that the location of the measurement points should be based on the model assumptions. In the other part, improvements must be made to obtain a satisfactory emission inventory for mobile and stationary sources.

Before the field program is designed and additional costs are incurred to improve the emission inventories, a sensitivity analysis of the models should be made. The sensitivity can refer to the extent to which the predictions of a model are influenced by a variation in a particular input parameter. Thus, we want to focus on the accuracy of the data used and the sensitivity of the model to variations (or uncertainties) in input data. It is important to determine the magnitude of sensitive parameters as accurately as possible. Little effort should be expended on improving the accuracy of relatively insensitive parameters. Sensitivity analyses (5) made on the SAI airshed model indicate that wind speed, mixing depth, radiation intensity, and emission rates are the most sensitive parameters. A sensitivity analysis of DIFKIN (6) indicated similar results, but also illustrated that the initial concentrations of HC and NO were sensitive parameters. Once we have an indication of what input parameters are most sensitive, it becomes a problem of designing a program to obtain quality inputs with minimal costs.

The following process describes the program followed by the California Department of Transportation to provide the highest quality data for use in regional photochemical models. This department was the lead agency in coordinating and completing the tasks described below.

Study Area

Defining the study area is the first task that must be completed before acquiring a data base. The inputs into regional modeling require the expertise of multidisciplinary groups and agencies. To resolve any conflict in defining the study area requires consultation with local planning agencies, air pollution control districts, state air resources board, EPA regional office, FHWA regional office, National Weather Service, and U.S. Department of Transportation. A multidisciplinary group can ensure that the boundaries of the study region provide for a common base line to include input of meteorology, pollutant emissions, and local land use plans. A group decision eliminates possible challenge as to the appropriateness of the selected region.

Emission Inventory

The next step is to obtain an accurate up-to-date emission inventory for mobile and stationary sources. Because the sensitivity analysis indicates that emission from mobile sources is an important parameter, justification within the California Department of Transportation was given to authorize expenditures to obtain the best state-of-the-art data.

Within the department, a computer program was developed to calculate vehicular emissions by using transportation simulation (7) models and a vehicular emission model (8). Both of the models were interfaced, and emissions were calculated for each link as a function of speed and then aggregated into grid emissions. The emissions were based on trip type, i.e., home to work, home to other, and so on. The emission model was based on the latest data available from EPA and ARB. The emission factors included the latest information on emission standards for light- and heavy-duty vehicles, speed adjustment factors, deterioration factors, vehicle mix distribution, and kilometers traveled per vehicle type for conditions in California. In some cases, the transportation simulation model was recalibrated based on more recent vehicle counts to reflect the changes in travel behavior caused by increased gasoline prices. This effort was felt to be essential in updating the vehicular emission inventory.

The latest update in aircraft emissions was obtained by contacting local airports in regard to the latest schedules of departures and arrivals. The latest aircraft emission factors available from EPA (9) were used to calculate the emissions. In one urban area, the local air pollution control district provided the updated aircraft emission inventory.

To obtain the updated stationary emission inventory, we held several meetings with local air pollution control districts. The results of the sensitivity analysis showed that stationary emissions are a sensitive parameter and that their best estimates for stationary emission would be required to obtain the best results. In most cases, unfortunately, the air pollution control districts provided inventories that were 2 years old until later inventories are updated and completed.

In the development of the emission inventories (mobile and stationary) it is strongly urged that the Universal Transverse Mercator (UTM) system be used to geocode both vehicular and stationary source inventories to ensure that emissions are allocated to the proper grid squares within the study region.

Field Monitoring Program

The next step is to design a field monitoring program to collect an aerometric data base. This data base has a dual purpose: (a) establish an input data base to describe the typical and worst day meteorological conditions and (b) establish a data base to compare predicted concentration with actual measured data. This design made use of all existing sources of data that were located with proper exposure based on the assumptions of the models.

To supplement the existing sources, the department used what instrumentation it had available and designed a new field air monitoring program. In the design of the field monitoring program, the following persons were consulted: air pollution control district meteorologists, meteorologists of ARB, consultants from the University of California, regional meteorologists of EPA, and meteorologists from the National Weather Service.

This team of experts decided where to locate surface wind stations, pibal release points, radiometers, additional ground air monitoring stations, and aircraft flights to measure temperature and air quality aloft. These instruments were located to best represent the temporal and spatial behavior of meteorology and air quality for the region investigated. The respective agency reduced and provided hourly average data that could be used for model inputs. All information was then coordinated by the transportation department and edited for final input into the models. The field monitoring program was designed to cover the primary and secondary pollutant seasons. For California this corresponds to the months of December through February for the primary pollutants and May through October for the secondary pollutants. Sampling continuously through these months should provide sufficient data to examine model predictions for comparison with observed data over a wide range of meteorological conditions and air quality concentrations. The estimated cost for the Sacramento study (based on California rates) for equipment (wind stations, bag samples), 3 air quality trailers, labor for data acquisition, and data analysis and model verification was $200,000. This cost covered sampling in the Sacramento area (40×40 square kilometers or 25×25 square miles), which is flat and has no local terrain effects and no major point sources. In areas where terrain effects alter surface winds and major point sources exist, such as in San Diego, additional wind stations and air monitoring stations are required and increase the cost considerably. The point that we emphasize is that to collect an aerometric data base for regional air quality modeling for a relatively small urban area requires a major effort in equipment availability and initial expenditures. Unless these data are available, it is not possible to use regional models with any degree of confidence (assuming that the emission inventory is available).

Institutional Constraints

To resolve the institutional constraints as previously described, the transportation department has 2 contracts: one with System Applications, Inc., and the other with General Research Corporation (GRC). The contract with SAI is to provide a working computer program with an expanded grid (50×100) to be run on the CDC 7600 computer. The contract also requires that a user documentation manual be prepared and that formalized training for department personnel be provided. Similarly, the contract awarded to GRC is to convert the DIFKIN model to the IBM 370/168 computer system with the expanded grid and to provide a training course. The total price of both contracts required an initial investment of approximately $100,000.

IMPLEMENTATION OF URBAN AIR QUALITY MODELS

The transportation planners and engineers have 2 types of air quality models from which to choose: grid model and trajectory model. As previously mentioned, in the grid model the airshed or study region is divided into a 3-dimensional grid, each cell being perhaps 2 km (1.2 miles) on a side and a few hundred meters high. The grid is then used as a basis for the numerical integration of the conservation-of-mass equation. In the trajectory approach, a hypothetical column of air is followed through the region as it is advected by the wind. Pollutants are emitted into the column, and chemical reactions take place within the column. Based on our experiences, both modeling approaches have the following advantages and limitations depending on the application.

Advantages of a Trajectory Model

1. The model is applicable for project level analysis. Figure 2 shows this application for a given highway project. For this application, the proposed highway was divided into 3 equal segments. The air parcel began over the ocean and eventually reached the segment 1 at 7 a.m. The path of the trajectory is indicated by path ABCDEFG. The actual path of the trajectory continues along the path H . . . P. The grid size is 3.2×3.2 square kilometers (2×2 square miles). Pollutant concentrations are predicted along the trajectory only.
2. The model can locate sources that produce hot spots for pollutant emissions.
3. Pollutant concentrations can be predicted in valleys because of the ability of the trajectory model to simulate air movements in valleys by using an air parcel approach.
4. The model is applicable to areas where terrain affects surface winds.
5. For a given trajectory, the model is computationally efficient and can be run on most computers at a reasonable cost.

Limitation of a Trajectory Model

1. The model is not directly applicable for convergent or divergent wind flow fields.
2. The model is not applicable where vertical wind shear is an important consideration.
3. The model is not applicable for transportation systems planning because of the numerous trajectories required to locate hot spots or areas where high concentrations occur.
4. The trajectories calculated are sensitive to the exposure of wind stations; therefore, surface wind data used as input must be consistent with model assumptions.
5. It is difficult to directly compare the trajectory model prediction of air concentrations at a given location or grid with the hourly National Ambient Air Quality Standards.
6. Large volumes of input data are required.

Advantages of a Grid Model

1. The model is applicable for system planning to determine the interrelations of land use, transportation, and air quality. Figure 3 shows the typical output for spatial concentrations of O_3 in pphm for the Los Angeles area.
2. The model is applicable to areas where terrain effects alter surface winds.
3. The model is applicable to areas where a convergent or divergent wind flow field exists.
4. The model is applicable for areas where wind shear is important.

Limitations of a Grid Model

1. It is expensive to run simulations on most computer facilities.
2. The model is not applicable to project-level analysis because of the expense in running the model.
3. The numerical solution of the partial differential equations introduces artificial diffusion problems and inaccuracies in the output if model runs simulate more than 10 hours.
4. Large volumes of input data are required.

Conclusions

Clearly, transportation planners and engineers must decide on the type of problem they

Figure 3. Typical output from SAI airshed model for Los Angeles.

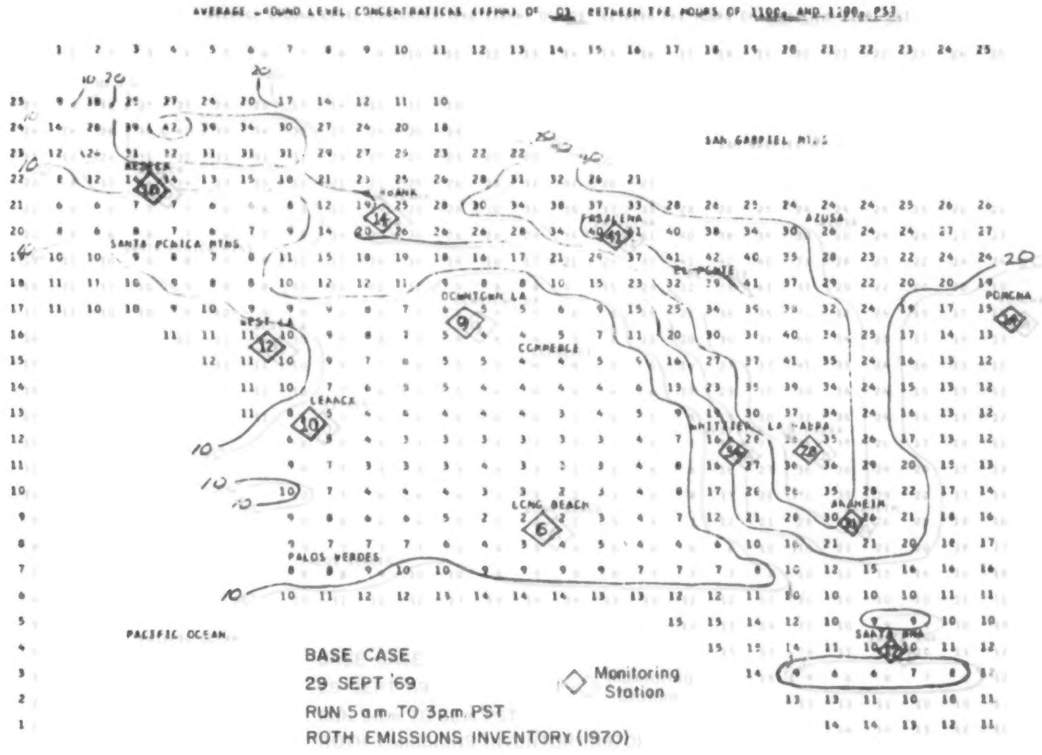
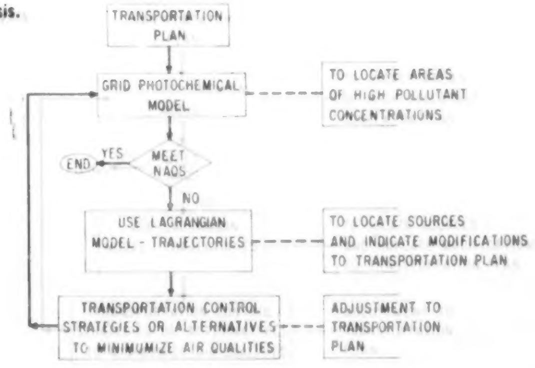

AVERAGE GROUND LEVEL CONCENTRATIONS (PPHM) OF O3 BETWEEN THE HOURS OF 1100, AND 1200, PST
SAN GABRIEL MTNS
SANTA MONICA MTNS
PASADENA
AZUSA
EL MONTE
DOWNTOWN LA
WEST LA
COMMERCE
LENNOX
WHITTIER
LA HABRA
LONG BEACH
ANAHEIM
PALOS VERDES
POMONA
SANTA ANA
PACIFIC OCEAN
BASE CASE
29 SEPT '69
RUN 5 a.m. TO 3 p.m. PST
ROTH EMISSIONS INVENTORY (1970)
Monitoring Station
10
20
40

Figure 4. Flow chart for systems analysis.


TRANSPORTATION PLAN
GRID PHOTOCHEMICAL MODEL
TO LOCATE AREAS OF HIGH POLLUTANT CONCENTRATIONS
MEET NAQS
YES
END
NO
USE LAGRANGIAN MODEL - TRAJECTORIES
TO LOCATE SOURCES AND INDICATE MODIFICATIONS TO TRANSPORTATION PLAN
TRANSPORTATION CONTROL STRATEGIES OR ALTERNATIVES TO MINIMUMIZE AIR QUALITIES
ADJUSTMENT TO TRANSPORTATION PLAN

want to evaluate and consider the possible trade-offs in modeling approaches. The user must select the model that is most cost effective for the desired application. The California Department of Transportation at present feels that both modeling approaches should be integrated in their application for transportation planning. First, the grid model is applied to evaluate the air quality of a proposed transportation plan. Using a grid model enables one to locate areas of high pollutant concentrations. Once the hot spots are located for a certain meteorological condition, a backward trajectory is then made by using a trajectory model to locate the respective emission sources in grids that cause the high concentrations. Next, a modification for the transportation plan is made to reduce the areas or grids of high pollutant emissions by perhaps considering spatial, temporal, or modal alternatives. Finally, the grid model is rerun to see whether the modifications to the transportation plan have reduced the hot spots and have not necessarily affected or altered the air quality in other areas. This process is repeated until a trade-off is reached. Figure 4 shows the use of the grid and trajectory photochemical models for systems planning.

Both modeling approaches have the common problem of requiring a large input data base, which initially is expensive to develop. Even with this initial investment to operate trajectory or grid models, transportation planners and engineers should consider the other alternative modeling approach available to them: rollback. A careful examination of whether rollback can evaluate spatial alternatives of emissions and their effect on quality will clearly indicate it cannot. Regional photochemical modeling is, at present, the only approach to provide rational answers to the complexity of today's problems. Confidence in any model can be achieved only by comparing predicted concentrations with observed data.

SUMMARY

This report discusses from the user's point of view the applications of regional photochemical models to assess the interrelations of land use, transportation, and air quality planning. It discusses the problems with using existing emission and aerometric data and presents solutions to remedy these problems. Institutional constraints to running computer simulation models on various computer systems are discussed. The advantages and limitations of trajectory and grid models are discussed for transportation systems analyses.

ACKNOWLEDGMENT

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Discussion

Alan Eschenroeder, Environmental Research and Technology, Inc., Santa Barbara

It is appropriate that Ranzieri and Shirely discuss at length problems of data acquisition for providing input to models. In this discussion, the counterpoint of solutions to these problems will be emphasized. Although these comments are from a developer's as well as a user's point of view, it should be noted that it is not my intention to endorse in a wholesale fashion or defend for all purposes the application of regional photochemical models.

Computer simulations, graphs, and formulas that may be called air quality models provide a vast array of possibilities on different levels from which to attack the problem of forecasting long-range trends in air quality as a function of emissions. Mathematical formulations that relate long-term averages to short-term averages or that relate air quality to meteorological variables are models of a sort; however, the term "air quality models" as defined here will be those means of evaluating emission control strategies.

DATA BASE

From a philosophical point of view the quality of the data base and the quality of the model formulation must not be confused. It is an oversimplification to say that a model does not perform well because of unknown uncertainties in the input data. Likewise, more precise statements than those made previously regarding the meaning of sensitivity can be formulated. For example, if it is found that the buildup of photochemical oxidant is extremely sensitive to the choices of nitric oxide flux at the ground, then we have encountered a manifestation of the extremely fast reaction of nitric oxide with ozone. In this example, it is incorrect to say that something is amiss with the model formulation because of a high degree of sensitivity. A more useful interpretation of this finding is that we must know the emission data base with relatively good accuracy for nitric oxide emissions if we are to predict oxidant buildup with any degree of confidence by using any model that captures the true chemistry.

The concern about nonstandard grids that is expressed by the authors is a real one in practical studies. Invariably the planning agencies, their consultants, the transportation agencies, and the environmental control agencies have slightly different views toward methods of data storage. A continued push is being made toward the application of Universal Transverse Mercator grid systems for the wide variety of emission-related data needed for inputs in photochemical diffusion models.

Probably the single most significant input feature for these models is an accurate space and time distribution for emissions of all primary pollutants. Standard data bases now have these emissions by county and not by grids as implied by Ranzieri and Shirely. We have found that these aggregated statistics may be geographically distributed according to land use maps with grid overlays. The output accuracy of transportation network flow simulations is really a problem separate from air quality modeling; however, it is one that must be considered by transportation planners for a variety of purposes including environmental quality predictions. As indicated later by the authors, computer packages are available for distributing the vehicle movement statistics from transportation simulations to rectangular or square grids used for air quality modeling. This is another area where the authors place more emphasis on the problems than on the solutions.

Although valid application of air quality models depends on truly representative meteorological and air quality data, there are very few cases where this will be available. The authors leave the reader with the dilemma that none of the data is good enough to use in existing models and that the alternative of rollback estimates is also unacceptable. Two messages should emerge from this dilemma: (a) Agencies that collect the data should be encouraged to exercise greater care in siting and measurement, and (b) models that can tolerate corrupted data should be developed for the near term.

In cataloging the data base problems, the authors give only slight emphasis to one of the largest outstanding problems for the modeling of photochemical oxidant regardless of what type of coordinate frame is used for a photochemical diffusion model. That problem is the detailed hydrocarbon inventory needed by the so-called second-generation photochemical diffusion models. At the present time it is difficult enough to obtain geographical and time distributions of reactive hydrocarbon emissions. The newer model versions, however, require an allocation of the reactive hydrocarbon emission into chemical classes such as paraffins, olefins, aromatics, and oxygenates. No control agency maintains files of such finely broken down hydrocarbon inventories. Nevertheless, there is a way out of this problem too. That is to consult some of the recent literature on reactivity assessments that gives rather detailed compound class breakdown to emissions from different types of pollutant sources. These approximate distributions can be folded in with aggregate reactive hydrocarbon inventories to obtain the needed distributions for future modeling.

APPLICATION OF EXISTING MODELS

The authors make repeated reference to comparison of model predictions with "real-world measurements." The existence of recently completed and ongoing field-measurement programs seems to be totally overlooked. Many millions of dollars have been spent by the California Air Resources Board in surveying 3-dimensional pollutant gradients, in tracing the movement of air masses in California air basins, and in measuring the composition as well as rate of appearance of photochemical aerosols. The Coordinating Research Council in conjunction with the National Oceanic and Atmospheric Administration and with the U.S. Environmental Protection Agency has completed the Los Angeles Reactive Pollutant Program, which provides an extensive data base designed for the verification of models. For the past several years and at the present, EPA is conducting the Regional Air Pollution Study in St. Louis expressly designed for the purpose of providing a validation data base for regional air quality models. In view of these efforts, it cannot be said, therefore, that "there has not been a great deal of attention given to measurement programs to provide input to verify regional photochemical models."

This comment is not intended to say that all the problems are solved, because in many cases measurement programs designed for model validation have not followed the statistical rules of experimental design, but rather have been constrained by logistical necessities. This means that future evaluation studies of models will still be hampered by data sample limitations; however, the scope of the measurements in the present round of field programs is so great that testing will now be possible for portions of models that have gone unchecked until now.

The outcome of these verification tests for different regions must be a set of performance parameters that can be applied to any model. The user can select the model on the basis of how well certain performance parameters are met. Naturally it is not the optimal solution to use the model with the highest degree of accuracy for all applications. Many cases of evaluation of future alternative decisions require a rank ordering or comparison rather than a specific calculation of a concentration level. Other cases require the probability of exceeding a certain threshold pollutant level rather than the complete computation of an ensemble of conditions.

It is difficult to compare costs in operation of models unless it is done in a rather gross sense. When actual dollar values are quoted, they must be carefully qualified by answering the question "costs to whom?" How many control agencies or transportation planning groups have access to CDC 7600 or STARR computer systems? The appeal for rewriting computer programs to increase efficiency is a good one and should be implemented by using recently developed numerical integration algorithms. In the category of other issues to be resolved before using regional photochemical models, there is now a substantial collection of aerometric data bases against which model assumptions can be tested. Again it should be emphasized that the fidelity of a model is not measured by its sensitivity to input data. In the example given previously, high degrees of sensitivity actually indicated a physical or chemical reality rather than a flaw in the mathematical formulation of the model. Commenting specifically on the sensitivity parameters discussed in the paper, it should be noted that grid models such as those developed by SAI and by Environmental Research and Technology, Inc. (ERT), depend on accuracy of initial conditions and edge conditions in addition to wind speed, mixing depth, and other parameters indicated in the paper. Lagrangian models such as DIFKIN exhibit this sensitivity in the assignment of initial concentrations. Because of the interchange of time for space, the need for accuracy in edge conditions translates into a need for accuracy in initial conditions.

Some of the limitations in both trajectory and grid models can be circumvented by careful applications and modifications. For example, vertical velocity modifications in the trajectory model will render it applicable for convergent or divergent flow fields. Shear corrections currently incorporated permit an accounting for this physical effect. The use of trajectory models for systems planning will be possible by using the multi-trajectory grid version of atmosphere reaction and transport simulation (ARTSIM) now under development at ERT. It is true that both types of models are sensitive to the exposure of wind stations and that surface wind data used as input must be consistent with model assumptions.

Regarding limitations on grid models for project level analysis, a limited portion of the grid may be treated for project level analysis at much lower expenditure of computer costs. The numerical problem of artificial diffusion has been overcome by the Egan and Mahoney code using conservation of moments that allows subgrid scale elements of contaminant to be treated in the advective portion of the program. Finally, both types of approach will benefit from more rapid numerical integration techniques that are being introduced by several groups.

IMPROVEMENTS IN THE MODELING ART

As mentioned in the previous sections, a number of features have been introduced to upgrade existing models. Even after this occurs, however, we are still faced with the dilemma of using either a relatively complicated physical-chemical formulation to predict oxidant levels or an inadequate data correlation called rollback. Up to now there are few available intermediate solutions that relate emissions to air quality (recall the cautions in the introduction regarding statistical models relating air quality to nonemission variables).

What is needed then is the invention of a new model that can be operated with existing data that may be insufficient for the photochemical diffusion models. The objective of such a model would be to relate emissions to air quality in only the degree of refinement required for evaluating emission control strategies. Very specifically this translates into a requirement to predict the number of violations of the National Ambient Air Quality Standards (NAAQS) and not the case-by-case or hour-by-hour prediction of concentrations at every point in an airshed. Another objective is that the model content be expressible in a simple enough algorithm that control agencies and transportation planners who possess little specialist training in meteorology and chemistry can use the models.

An approach to this problem can be found in the use of cluster analysis. In this form of analysis a dependent variable is classified into clusters as determined by values of an independent variable. For example, we might take individual hours that violate the NAAQS and designate them with a V for violation, then take those hours that do not violate the NAAQS and designate them by an N for nonviolation. The next step might be to plot Vs and Ns with a graph of mean daily temperature versus emissions into an air parcel arriving at each particular hour. If this is a good choice of independent variables, we will have 2 clusters of Ns and Vs that show little overlap. This degree of knowledge is important for designing control strategies because it tells us what causes are in operation to bring about violations or nonviolations. This is one example of a type of model that may be developed to supplement rollback or diffusion modeling.

CONCLUDING REMARKS

Although data base problems exist, they are not insurmountable. Uniformity has been attained in many cases where commonality in land use, traffic, and resource inventories is achieved. Meteorological and air quality data bases are growing, and the awareness of correct sampling or calibration procedure is developing in many agencies. Although existing models may be adapted to special cases of either transportation project studies or system studies, their degree of complexity will be growing as physical and chemical improvements are introduced. The so-called second-generation models require levels of input data far beyond those that will normally be available. Therefore, they must be looked on as testbeds for concepts in air pollution control and for interpolating or projecting details in air quality distribution such as "hot spots" with respect to sources or receptors. General control strategies will probably use cruder models than these highly refined finite difference computer simulations. The crudeness will not extend to the level of simple rollback, but rather will include the basic chemical and meteorological factors influencing air quality in the future. We wholeheartedly agree that the rollback procedure cannot provide answers to problems of predicting concentration in the future. These strategies will involve, in some cases, unusually severe economic and social dislocations; therefore, we will strive for timely and reliable predictions using information that is typically available from existing data sources.

WORKSHOP 2

NONREACTIVE MODELS

ISSUES IN NONREACTIVE MODELS

Jesse R. Chaves, Federal Highway Administration, Baltimore

In assessing transportation-related air quality impacts, we are aware of the numerous changes that have recently occurred and continue to take place. Within the past few years, many new analysis techniques, methodologies, and models have been introduced. Older models have been refined or enhanced. Field validation studies have been performed. Users and researchers have had the opportunity to gain additional experiences with the implementation of these techniques. During this 2-day workshop, it was possible to cover in depth only a limited number of the models and methodologies that are currently available for microscale and regional analysis.

The principal objective of Workshop 2 was to provide the latest information on nonreactive models and methodology to those persons responsible for carrying out air quality impact assessments at both the microscale and mesoscale levels. Models for reactive pollutants were discussed in Workshop 1.

Gaussian line source models have played an important part in assessing air quality impacts of proposed highway projects in connection with the preparation of environmental impact statements. Many are familiar with or have used the line source model developed several years ago by the California Department of Transportation. Ward and Ranzieri provide an update on the modifications and additional field validation that have resulted in a new version of this model called CALINE2.

Microscale numerical models, sometimes referred to as conservation-of-mass models, are probably not so familiar to the average user, nor have they been so extensively used as have the Gaussian models. Sontowski presents the theoretical basis of numerical models and discusses how they differ from the Gaussian formulation. His discussion includes the proprietary and nonproprietary models that are currently used.

Downey describes results of a statistical comparison of 13 models using synthetic data samples. The lack of a reliable air quality data base did not permit the validation of the accuracy of these models, but these comparisons may assist potential users in the selection of models for their work.

Patterson discusses a relatively new methodology for estimating concentrations of carbon monoxide near signalized intersections. This procedure takes into account differences in emissions resulting from motor vehicles operating in various modes on a street or highway.

Ellis, Dabberdt, Kozlowski and Caruso, and Nash are all concerned with models that have been used for urban regional analysis. Ellis relates the experiences of one state highway agency in implementing the APRAC-1A urban diffusion model. Several modifications that have been made are described. Dabberdt, a representative of the firm that originally developed the model, comments on this paper. A regional emissions model called SAPOLLUT was sponsored by the Federal Highway Administration, and Kozlowski and Caruso describe recent improvements and modifications to this model. Nash, a user of SAPOLLUT, comments on this methodology and relates experiences with it in Virginia.

Williams explains EPA's program for measuring motor vehicle emissions and describes the new methodology and the reasons behind it. The important topic of

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monitoring ambient air quality is discussed by Palmieri, who gives practical advice based on the experience gained in setting up a monitoring program by one state transportation agency.

The following questions were posed at the beginning of the workshop, and were addressed in the discussions during the 2-day period.

1. What accuracy can be reasonably expected from available microscale Gaussian and numerical models under optimal conditions?
2. Are microscale models sufficiently validated so that users can apply them with reasonable confidence in most situations? How can we judge whether a model is adequately validated?
3. Are microscale models available that can be applied in areas of rough topography, in city environments, and to highway interchanges?
4. Under what circumstances will users need to validate models they plan to use? What would this entail?
5. Have microscale models been challenged either by air quality control agencies or in litigation? If so, how do we avoid such challenges?
6. What can we really find out from model comparisons? Can we use a properly validated model to determine the accuracy of another model?
7. Should some group or agency compile a list of "acceptable" or "approved" microscale models? Would this be feasible or desirable? Do we have an adequate air quality data base to do this?
8. Where should future research and development efforts be concentrated in microscale model development? Do we need to concentrate on improving either existing Gaussian or numerical models or both?
9. Have we reached a stage in microscale model development in which the potential accuracy of the models exceeds the reliability and accuracy of the best available input data such as estimates of future traffic volumes, speeds, emission factors, and meteorological parameters? If the reliability of input data is the weakest link, are we not faced with a basic dilemma?
10. What methodologies are currently available for estimating present and future carbon monoxide emissions and concentrations near signalized intersections? How reliable are the estimates using these methods?
11. What mesoscale models are available that can be used for estimating the urban distribution of carbon monoxide levels for future years? Do these models provide sufficient spatial resolution so that they provide reasonable estimates of the 1-hour and 8-hour maximum background concentrations needed for individual project analysis? Do these models need to be validated? If so, can data from existing monitoring networks be used for validating background levels?
12. When can we expect EPA to officially promulgate supplement 5 of AP-42? How will this be done and by whom? How often can we expect AP-42 revisions to be made? Will contemplated revisions to supplement 5 be based on the same methodology? Can users expect from EPA documented computer programs to assist in implementing supplement 5 and subsequent revisions? Will transportation agencies be able to provide the detailed data required by supplement 5 to compute composite emissions?

CALINE2: AN IMPROVED MICROSCALE MODEL FOR THE DIFFUSION OF AIR POLLUTANTS FROM A LINE SOURCE

*Charles E. Ward, Jr., and Andrew J. Ranzieri, Transportation Laboratory,
California Department of Transportation*

Compliance with the National Environmental Policy Act (NEPA) and the California Environmental Quality Act (CEQA) requires that an air quality assessment be included as part of the environmental impact report prepared for proposed transportation projects. In addition, the Federal-Aid Highway Act and the Clean Air Act of 1970 require air quality analyses for proposed transportation systems.

Transportation agencies must be able to estimate changes in air quality within the highway corridors to comply with these laws and their associated regulations. The highway corridor is defined as the region extending from the vehicular source of the pollutants to the point where ambient pollutant levels are again reached. The primary pollutants emitted from motor vehicles are hydrocarbons (HC), carbon monoxide (CO), nitrogen oxides (NO_x), and particulates. Lead is the major form of particulates, but catalytic convertors have caused sulfate particulates to be of increasing concern. Reactive hydrocarbons (RHC), which are a major proportion of the total vehicular-emitted hydrocarbons, combine in the presence of sunlight with nitrogen oxides to form smog.

Photochemical formation of smog is a large-scale phenomenon and should be analyzed on a regional basis. For a corridor analysis, carbon monoxide is suitable as a tracer pollutant to define air pollutant dispersion because of its relative inertness in the photochemical smog process. Lead and sulfate particulates are not yet considered because of the lack of quantitative data on emission rates and dispersion characteristics. Line source computer models have been developed during the past few years to simulate the dispersion of carbon monoxide within the highway corridor. The California Department of Transportation model, CALINE2, has been so named because it is the second major version of the California line source dispersion model. The first version is described in the air quality manual (1).

Included in this paper are a discussion of the Gaussian dispersion theory, the mathematical assumptions of CALINE2, a sensitivity analysis, and a comparison of the CALINE2 predictive capabilities with observed data.

MATHEMATICAL ASSUMPTIONS

General Gaussian Assumptions

Gaussian Dispersion

The Gaussian dispersion equations, as described by Turner (2), were developed to describe the dispersion of an inert pollutant from a point source with a constant emission rate. The equations assume that the concentrations of pollutants follow a normal distribution in the horizontal and vertical directions. Figure 1 shows the dispersion in a typical case and the coordinate system used. The general form to describe the Gaussian diffusion equation is

$$C(x,y,z;H) = \frac{QF}{2\pi\sigma_y\sigma_z\bar{u}} \left\{\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\right\} \left\{\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]\right\} \tag{1}$$

where

C = concentration,
x,y,z = receptor location in 3-dimensional space,
H = effective stack height,
Q = source strength,
σ_y, σ_z = horizontal and vertical dispersion parameters,
$\bar{u}$ = mean wind speed, and
F = conversion factor to change input units to output units.

The edge of the Gaussian plume is defined as the point in the y-z plane where the pollutant concentration is a tenth that of the centerline. This point is at a distance of 2.15σ from the centerline. Perfect reflection of the plume is assumed when it contacts the ground surface. This assumption is incorporated into equation 1 by creating an imaginary point source that is an undersurface mirror of the actual source. The (z + H) term is related to the vertical dispersion downwind from the actual point source, and the (z - H) term is related to the vertical dispersion from the imaginary source. Equation 1 only calculates the concentration from the source itself. It does not include the upwind ambient level.

One of the shortcomings of Gaussian dispersion as stated in equation 1 is its inability to handle trapping of pollutants by the "lid" of an elevated inversion. However, in the microscale (highway corridor) region for which CALINE2 was developed, the vertical dispersion of pollutants from a line source usually does not reach the inversion base height. The basis of CALINE2 is that equation 1 is modified to accommodate a line, rather than a point, source. This modification is described in detail in a later section.

Atmospheric Stability Classes

The surface-layer stability of the atmosphere can be classified into separate Pasquill stability categories according to meteorological parameters as suggested by Turner (2). Pasquill developed a series of graphs for the dispersion parameters (σ_y and σ_z in equation 1) as a function of his stability classes and the downwind distance x from the source (Figures 2 and 3).

Unfortunately, the Pasquill dispersion parameters shown in the graphs are only valid for downwind distances from 0.1 to 100 km. Many line source impact analyses are concerned with receptors closer to the highway than 0.1 km, especially in the right-of-way range of 15 to 50 m. Modifications to the dispersion parameter curves to handle downwind distances less than 0.1 km are discussed in a later section.

In addition, Pasquill's original research was conducted in flat, open country or rural areas. It has been found that his stability classes do not adequately describe the atmospheric turbulence encountered in urban areas or rough or forested terrain (2, 3). Neither the aerodynamic roughness height nor the unnatural energy imbalance created by man-made surfaces is incorporated in his dispersion parameter graphs. Although no attempt has been made to incorporate the higher turbulence encountered in urban areas into the stability parameters in CALINE2, as was done in other Gaussian models (3), stability class D (neutral) can be used in urban project analysis to account for this increased instability.

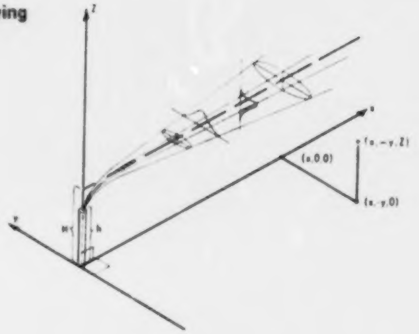


Figure 1. Coordinate system showing Gaussian distributions in the horizontal and vertical.

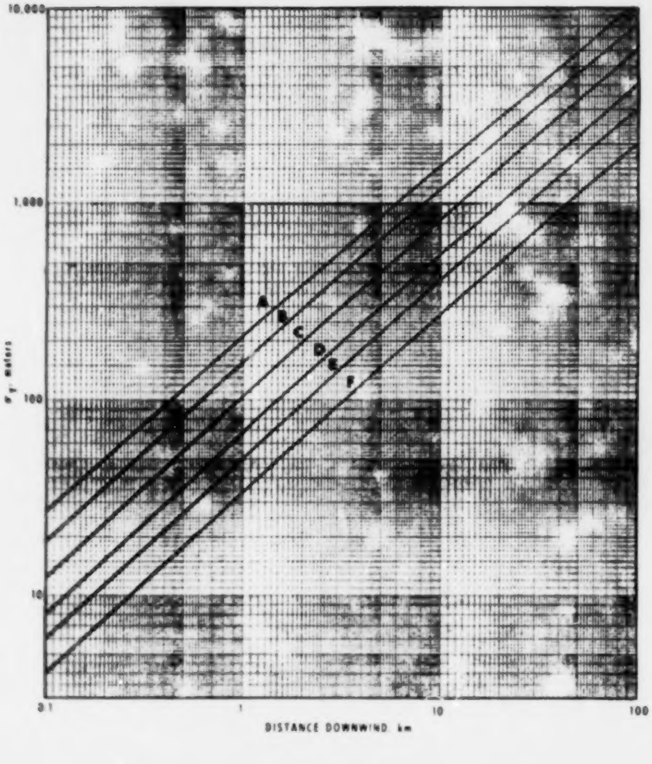


Figure 2. Horizontal dispersion coefficient σ_y as a function of downwind distance from the source.

Wind Shear

The wind speed within the atmospheric boundary layer varies from near zero at the ground surface to some finite free flow velocity at a height of around 500 m. This last figure is highly dependent on surface roughness characteristics and is closer to the ground for flat, even terrain and higher for central business districts with multistory buildings (Figure 4). The Gaussian dispersion equations do not incorporate the wind

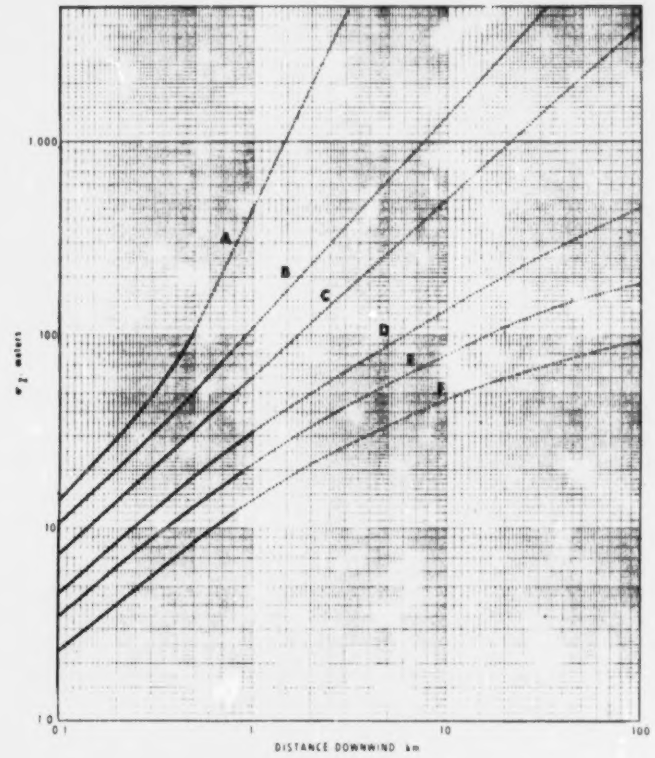


Figure 3. Vertical dispersion coefficient σ_z as a function of downwind distance from the source.

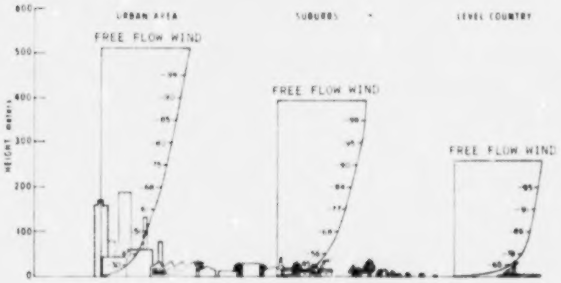

600
500
400
300
200
100
0
HEIGHT meters
URBAN AREA
SUBURBS
LEVEL COUNTRY
FREE FLOW WIND
FREE FLOW WIND
FREE FLOW WIND

Figure 4. Examples of wind shear with different size roughness elements (numbers are percentages of free flow wind).

shear. Rather, they assume a uniform vertical wind flow field with some mean wind velocity, $\bar{u}$, as shown in Figure 5, that is not influenced by surface roughness.

Aerodynamic Eddies

Physical objects in the path of a uniform wind flow field, such as buildings, highway viaducts, or street canyons, cause the flow to separate and form turbulence eddies. Cavities, areas of divergence, and areas of convergence form, which may disperse or concentrate pollutants, depending on the configuration and interaction of the different eddies.

For example, cavities formed in street canyons have been found to allow inadequate dispersion of pollutants under otherwise turbulent atmospheric conditions (4). Aerodynamic eddies are not included in the Gaussian dispersion theory. Therefore, other means have to be sought to account for these important effects. One such approach is discussed later.

Gaussian Line Source Assumptions

Mixing Cell Concept

It was surmised that the physical movement of the vehicles on a typical line source, a highway, would create a well-mixed region surrounding the highway that would not be affected by surface atmospheric stability. To test this theory, the California Department of Transportation conducted a series of smoke plume dispersion tests on an abandoned airport runway north of Sacramento in 1972 (5). By observing and photographing the initial dispersion of smoke from sources placed in the tailpipes of test vehicles, it was determined that the theory was sufficiently valid. The plume studies indicated that the limits of the mixing cell are approximately equal to the width of the paved surface and twice the height of the vehicle. As a representative average of the vehicle mix, the vertical limit of the mixing cell was set equal to 4 m. The width of the mixing cell, which is also called the highway width, is determined by adding the width of all the lanes, up to the edge of traveled pavement, plus the median, and an extra distance equal to approximately 3 m on each side of the highway. This last is to account for the horizontal turbulence created by the mix of heavy-duty and light-duty vehicles. The same horizontal turbulence is assumed to create a well-mixed region across the median, as long as the median is less than 9.1 m wide. If the median is greater than 9.1 m in width, each direction will have to be simulated separately, as discussed later.

The mixing cell is used as a uniform, well-mixed pollutant source from which the pollutants are then dispersed downwind in a Gaussian manner. Figure 6 shows this concept and also shows how the ambient or base-line pollutant level has been excluded. It is assumed that the concentrations of pollutants within the mixing cell are unaffected by regional meteorological conditions because of the turbulence generated by the moving traffic. The mixing cell can be represented by a tunnel in which the air is thoroughly mixed.

Dispersion Parameter Modifications

To determine dispersion parameters for downwind x distances less than 0.1 km, we set the initial dispersion of a line source equal to that found at the edge of the mixing cell. Interpolative curves were then drawn between these points and the original Pasquill curves. From the empirical evidence of the smoke study, the initial vertical dispersion parameter was set at 4 m (Figure 7).

So that the individual project's width can be accommodated, the initial horizontal dispersion is found by dividing the highway width by the plume width constant, which equals 4.3. (Since the edge of the plume is at a distance of 2.15σ from the plume centerline, the plume width is twice this amount, or 4.3σ. Therefore, the plume width constant is 4.3.) The reason for this, which is more completely explained in a later section, is based on the fact that the horizontal dispersion parameter is only incorporated in the parallel wind equations. A point along an extrapolation of the stability class A curve as defined by Beaton et al. (6) (Figure 8) is found that corresponds to this initial horizontal dispersion, and the first portions of the other stability class curves are modified to begin at this point. For example, the horizontal dispersion parameter for stability class F is assumed to be linear (on a log-log plot) with downwind distance from the initial dispersion parameter of approximately 1 km, at which point it intersects the previously established curve. Figure 9 shows this situation for different highway widths.

Figure 5. Uniform vertical wind flow field.

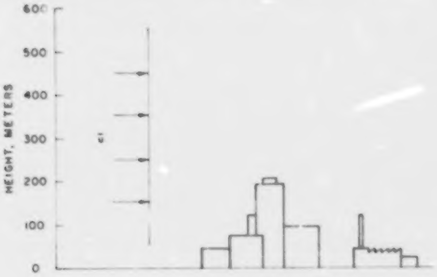
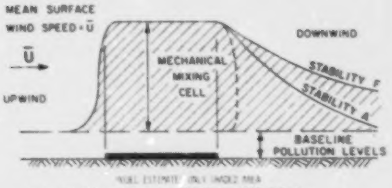


Figure 6. Mixing cell.


MEAN SURFACE
WIND SPEED = Ū
Ū
UPWIND
MECHANICAL
MIXING
CELL
DOWNWIND
STABILITY F
STABILITY A
BASELINE
POLLUTION LEVELS

MODEL ESTIMATES ONLY SHADED AREA

TOTAL POLLUTANT CONCENTRATION = BASELINE POLLUTANT LEVELS + POLLUTANTS GENERATED FROM HWYS.

Figure 7. Vertical dispersion parameters.

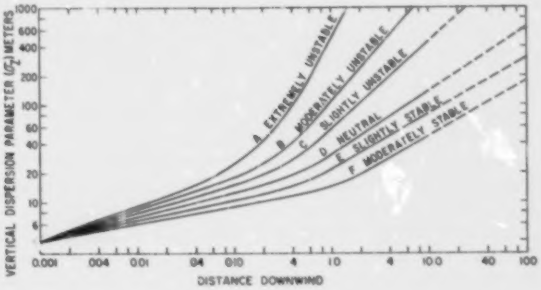


Figure 8. Horizontal dispersion parameters.

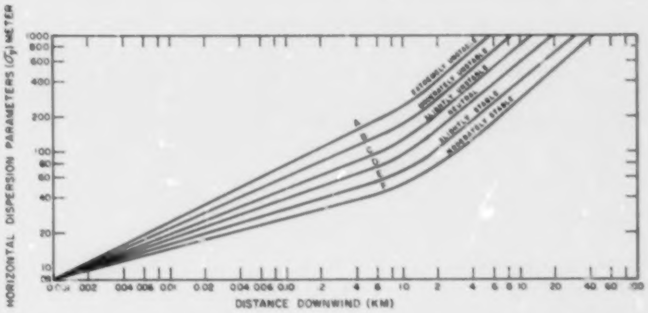
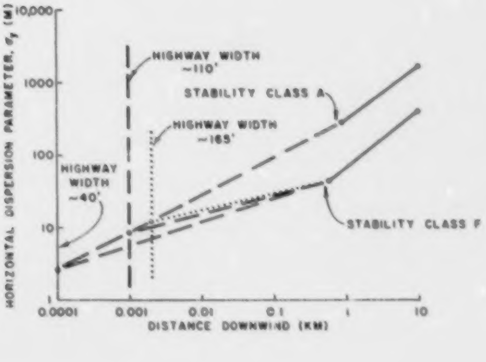


Figure 9. Modification of σ_y for variations in highway width.



Crosswind Line Source Equation

The dispersion of pollutants from an infinite line source with a perpendicular wind (90 deg) can be described by the following equation (6):

$$C_1 = \frac{Q_1F_1}{\sqrt{2\pi}\,\sigma_z\bar{u}}\left\{\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]\right\} \qquad (2)$$

where

Q_1 = VPH × EF,
VPH = vehicles per hour,
EF = emission factor, and
H = height of pavement above ground surface.

The subscript 1 on C_1, Q_1, and F_1 refers to the crosswind component of the pollutant concentration, line source strength, and conversion factor. Equation 2 is valid as long as the end of the line source is far enough away from the point being analyzed that end effects are unimportant. Figure 10 shows a display of the crosswind situation.

Parallel Wind Line Source Equation

When the wind is parallel to the highway alignment (0 deg), a buildup of pollutants occurs in the downwind mixing cell because an air parcel continues to amass pollutants as it travels along the highway. When the wind is parallel, the assumption can no longer be made that the highway has no width. The following equation is used to account for these factors:

$$C_2 = \sum_{i=1}^{\infty}\frac{Q_2F_2}{2\pi\sigma_{y_i}\sigma_{z_i}\bar{u}}\left\{\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_{y_i}}\right)^2\right]\right\}\left\{\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_{z_i}}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_{z_i}}\right)^2\right]\right\} \qquad (3)$$

where

$Q_2 = Q_1 \times W$, and
W = highway width.

The subscript 2 on C_2, Q_2, and F_2 refers to the parallel wind component of the pollutant concentration, line source strength, and conversion factor.

The assumption is made that a highway with a parallel wind can be approximated by the summation of a series of square area sources, each having the same source strength but a different distance to the receptor. The area sources themselves are approximated by virtual point sources. This last is why equation 3 is the same form as equation 1 for the summation. To agree with the infinite line theory of the crosswind case, the summation is made over an infinite distance downwind. However, the summation need be carried out only to a finite distance, which is dependent on stability class. At this distance, the contribution of pollutant from area sources located farther upwind from the receptor becomes negligible. Since this distance is only dependent on stability class, a scaling factor (Figure 11) for each class can be used to increase the calculated concentration from a short finite parallel wind segment to that for the infinite line source. The short finite segment has been determined as 0.8 km to allow the incorporation of different highway widths (and, thus, different σ_y curves) with minimal error while shortening the computer time necessary to make the reiterative summation. Figure 11 shows the mixing cell CO concentrations as a function of summation length and stability class.

A virtual point source is defined as a point source that has the same emission strength as the actual area source, is located at a distance upwind of the area source, and yields the same horizontal dispersion parameter as that at the upwind edge of the area source. To find the initial horizontal dispersion parameter of the area source, one divides the width of the area source (which is the highway width) by the plume width constant 4.3, which yields the σ_y for the upwind edge (2). The virtual distance corresponding to this σ_y is found on the horizontal dispersion curve for the appropriate stability class (Figure 9). The vertical dispersion parameter σ_z is assumed to follow the same virtual distance as σ_y. In other words, the virtual distance determined for σ_y is used to find the appropriate σ_z with the curves in Figure 7. Figure 12 shows the basic conceptualization of the parallel wind-virtual point source situation.

The virtual point source should theoretically be aligned with the centerline of the area source. However, this would presume that the concentration across the area source would follow a normal distribution, thereby disagreeing with the definition of the mixing cell. The mixing cell definition mandates a constant concentration throughout the area source. Essentially what has to take place to again agree with the mixing cell definition is that the axis of the virtual point source (the x-axis) has to be shifted toward the edge of the mixing cell. Shifting the axis toward the edge causes the normal distribution to be intersected by the mixing cell edge at a point closer to the mean of the distribution, yielding a higher concentration. The higher concentration is then said to be the concentration of the mixing cell, or area source. This shifting of the x-axis artificially imposes the mixing cell definition on a normal distribution. The shifting of the x-axis is incorporated in the y term of equation 3; i.e.,

$$y = y' + s \tag{4}$$

where

y' = horizontal distance from the edge of the mixing cell to the receptor, and
s = distance of the x-axis shift.

The distance s is found by solving equations 2 and 3 (the latter for only the first area source segment) for z, H, and unmodified y set equal to 0 (which is the location of the mixing cell), resulting in equations 5 and 6.

$$C_1(x,0,0;0) = \frac{2Q_1F_1}{\sqrt{2\pi}\sigma_z\bar{u}} \tag{5}$$

$$C_2(x,0,0;0) = \frac{2Q_2F_2}{2\pi\sigma_y\sigma_z\bar{u}} \tag{6}$$

Neglecting F_1 and F_2, since they are only conversion factors, and remembering that $Q_2 = Q_1 \times W$, we see that equations 5 and 6 differ only by a factor of $W/(\sqrt{2\pi}\sigma_y)$. Since the mixing cell concentrations for a crosswind line source and the first area source segment of a parallel wind line source should be the same, for given atmospheric conditions and roadway configuration, a factor of $(\sqrt{2\pi}\sigma_y)/W$ is required in the parallel wind equation (equation 6). Because the axis has to be shifted, this factor is assumed to be obtained through $\exp[-\frac{1}{2}(s/\sigma_y)^2]$. Therefore,

$$\exp\left[-\frac{1}{2}\left(\frac{s}{\sigma_y}\right)^2\right] = \frac{\sqrt{2\pi}\sigma_y}{W} \tag{7}$$

and

$$s = \sigma_y\left[-2\ln\left(\frac{\sqrt{2\pi}\sigma_y}{W}\right)\right]^{1/2} \tag{8}$$

For any given values of W and σ_y, s approximately equals the σ_y associated with the virtual point source. Therefore, the physical interpretation of the above mathematics is that the shifted x-axis lies between the actual centerline and the mixing cell edge, at a distance approximately equal to W/4.3 (the σ_y of the virtual point source) from the edge of the mixing cell.

Oblique Wind Line Source Equation

The consideration of a wind blowing at an oblique angle to the highway (0 deg < angle < 90 deg) is made easier by the fact that both the crosswind and the parallel wind equations are for infinite line sources. This similarity allows components of the 2 "pure" wind angle equations to be added via weighted vectorial coefficients.

Figure 13 shows that a wind $\bar{u}$ can be broken down into a crosswind component $\bar{u}$ sin ϕ and a parallel wind component $\bar{u}$ cos ϕ. However, the concern with CALINE2 is to find the pollutant concentration resulting from an oblique wind, and not the vector components of the wind. By the use of the trigonometric identity, $\cos^2\phi + \sin^2\phi = 1$, the concentration from an oblique wind was assumed to be equal to

$$C_3 = \sin^2\phi\, C_1 + \cos^2\phi\, C_2 \tag{9}$$

where the subscript 3 on C_3 refers to the oblique wind pollutant concentrations, C_1 and C_2 are as defined in equations 2 and 3, and ϕ is the acute wind angle. In this case, the trigonometric relation was used to functionally smooth the sum of the components from each of the pure wind angle equations. The preliminary verification study supports this assumption.

Source Height Adjustments

The H term in equations 2 and 3 is used to indicate a highway section that is depressed in relation to the surrounding terrain or at grade or raised above the terrain, as in a fill or viaduct section. Highway sections that are other than at grade are difficult to handle in a line source model because the Gaussian theory does not account for aerodynamic eddies, as discussed earlier.

The carbon monoxide data gathered in Los Angeles in 1972 (7), which included measured concentrations for 2 depressed sites up to 7 m deep, were used to develop a set of empirical ratios to approximate the nonuniform wind flow through a depressed highway section. By the use of multiple stepwise linear regression, the variables were determined that had the most correlation with the measured pollutant concentrations directly above the highway at the level of the surrounding terrain (8). The variables considered were traffic volumes, emission factors, wind speed, wind direction, pavement height, and Pasquill stability class. From the analysis, regression coefficients were determined that related the most significant variables to the carbon monoxide concentrations. The empirical equations for depressed sections are categorized by stability class.

For stability class A,

$$R = 10^{(-0.18164+0.01448H+1.439\times10^{-5}VPH+7.9\times10^{-4}\phi)} \tag{10}$$

For stability class B,

$$R = 10^{(0.21754+0.01431H-7.2\times10^{-4}\phi-0.02252\bar{u})} \tag{11}$$

For stability classes C through F,

$$R = 10^{(0.02019+0.0138H+4.98\times10^{-6}VPH-5.73\times10^{-3}\bar{u})} \tag{12}$$

where R = the empirical ratio, and the other variables are as previously defined. The empirical ratio R was derived from the CO concentrations measured at 1.2, 3.6, 6.1, 10.9, or 13.4 m, divided by the CO concentration at 1.6 m. All heights are heights measured above the pavement height, and not the height of the surrounding terrain. Any height above 1.6 m had an R value of less than 1, although the ratio at 3.6 m always had a value quite close to 1, reinforcing the concept that a uniform mixing cell exists. In a few cases, the aerodynamic eddies caused some increase of CO concentrations with height. These cases were excluded from the analysis and will be subjected to future research.

There is only one equation for stability classes C through F (equation 12) because insufficient data were obtained for stability classes E and F because of meteorological conditions. Until further data are gathered, the relation derived for stabilities C and D are assumed to apply to stabilities E and F.

A physical interpretation of the above equations is that an imaginary mixing cell is created at the level of the surrounding terrain and has a smaller source strength than the actual mixing cell on the highway below (Figure 14). Other than the decreased source strength, the imaginary mixing cell has all the characteristics of the original: the same dimensions, the same uniform distribution of pollutants, and so on. The pollutants in this imaginary mixing cell are then dispersed in the normal Gaussian manner downwind.

At this time, no attempt has been made to develop empirical equations to handle the raised highway section where aerodynamic eddies occur. At present, a raised section is simply considered as an elevated source whose pollutant emissions are dispersed downwind in the same manner as an at-grade line source using the Gaussian equation.

Summary of Assumptions

1. Gaussian (normal) dispersion of pollutants is in horizontal and vertical directions of plane perpendicular to wind direction.
2. A uniform wind flow field exists, with no vertical wind shear or aerodynamic eddies from uneven surface roughness.
3. No buildup of inert pollutants occurs due to elevated inversion conditions for microscale prediction of air quality.
4. No chemical reactions or gravitational settling occurs that affects the pollutant

Figure 10. Schematic of general Gaussian dispersion of pollutants from an infinite line source under crosswind conditions.

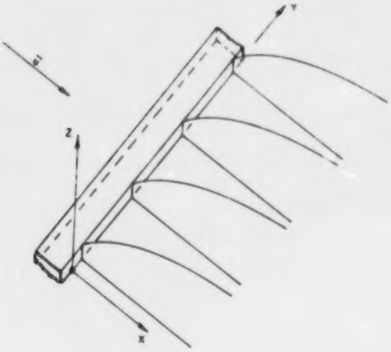


Figure 11. Mixing cell concentrations as a function of highway length parallel to wind.

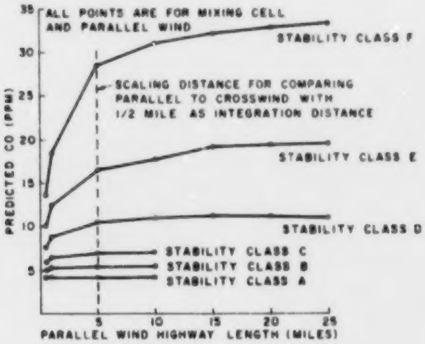


Figure 12. Schematic of general Gaussian dispersion of pollutants from first virtual point source under parallel wind conditions.

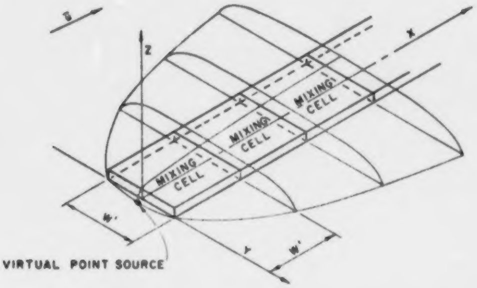

ū
Z
X
MIXING CELL
MIXING CELL
MIXING CELL
W'
Y
W'
VIRTUAL POINT SOURCE

Figure 13. Vector components of an average wind speed with an angle to the highway of ø.

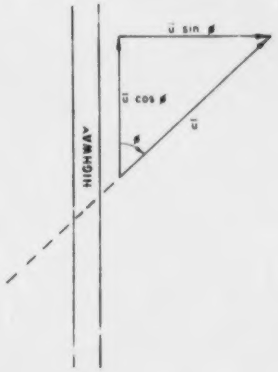

ū sin ø
ū cos ø
ø
ū
HIGHWAY

Figure 14. Imaginary mixing cell for depressed highway sections.

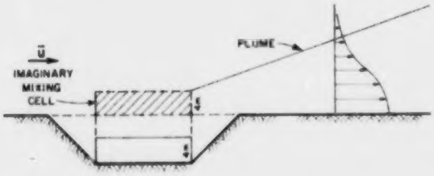
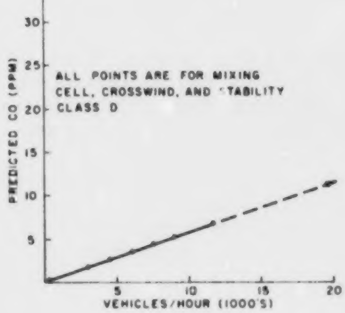

ū
IMAGINARY MIXING CELL
PLUME

Figure 15. CALINE2 sensitivity to vehicles per hour.



during the period of analysis.

5. Vehicles using the line source represent a continuous and constant source of emissions.
6. The initial vertical and horizontal dispersion of pollutants within the mixing cell is twice the height of the average vehicle (or 4 m) and a function of the highway width respectively.
7. Pollutants are uniformly distributed throughout the mixing cell region regardless of surface atmospheric stability conditions.
8. Perfect plume reflection occurs when the plume intersects the ground surface.
9. Parallel winds cause a buildup of pollutants.
10. A line source having a width W can be approximated by a series of square area sources with W-length sides, which can in turn be approximated by virtual point sources.
11. A finite highway segment can be approximated by "infinite" line source equations.
12. Pasquill stability classes and modified dispersion parameters adequately describe the turbulence of the atmosphere.
13. Predictions are only made above ambient levels.

DATA FORMAT ASSUMPTIONS

Time Interval

The CALINE2 line source model makes calculations of pollutant dispersion based on hourly averages only. This implies that the output is the concentration of carbon monoxide averaged during 1 hour. The constraints are that all data on which the calculations are based, such as the meteorology and traffic volumes, must be hourly values. Obviously, consistency must be maintained in the definition of the hourly average; i.e., if an hour is defined as the period of time between 30 min before 1 hour until 30 min before the next, this definition must apply to all variables.

Input Data Requirements

As input, CALINE2 requires the following:

1. Traffic volume, in vehicles per hour;
2. Average emission factor, in grams per kilometer or mile;
3. Hour's average wind speed, in kilometers or miles per hour;
4. Hour's average wind angle to highway, in degrees;
5. Hour's surface atmospheric stability class;
6. Average pavement height of the section under consideration, in meters or feet, in relation to the surrounding terrain;
7. Average highway width in meters, including median (if less than 9.1 m), all lanes, and 3 m on each outer side of the highway;
8. Receptor distance, in meters or feet, as measured in the perpendicular distance from the nearest outside edge of the traveled roadway lane plus 3 m; and
9. Receptor height, in meters or feet, in relation to the surrounding terrain.

The meteorological data should be as representative of the individual site as possible, which implies that the guidelines set forth in the meteorology manual (9) should be closely followed. One of the most important of these guidelines is that the meteorological measurements of wind speed and direction be made at 10 m above the surrounding canopy.

There are 2 constraints that must be observed when input data are acquired for the model. Since pollutant concentration is inversely proportional to wind speed, a decrease in wind speed causes a hyperbolic increase in the calculated concentration. As the wind speed approaches zero, the concentration approaches infinity. The lowest wind speed recommended in Gaussian models is 1 m/s, approximately 2 mph (6). A disproportionate increase in concentration occurs if the wind speed is allowed to go below 1 m/s.

The second constraint is that the empirical ratios for depressed sections were developed for sections 7.3 m below grade, as discussed in an earlier section. Since the model is only valid down to 7.3 m, it is not recommended that this model be applied to depressed sections greater than 9.1 m. (Based on our experience in monitoring CO along roadways, we feel that the empirical ratios for depressed sections can be extrapolated up to 9.1 m and still provide reasonable estimates of CO.)

SENSITIVITY ANALYSIS

Definition of Sensitivity Analysis

Mathematical computer models are used in the decision-making process because they are capable of describing the complex physical transport and diffusion of air pollutants. They require little time to make the calculations. However, it is sometimes difficult to conceptualize the interactions of a complex numerical model of a real-world process. Since each small part of the model has to be developed separately and later interfaced with the other parts, synergistic and nonrealistic situations develop internally when the model is used. Therefore, sensitivity analysis must be used on a complex model to determine those inconsistencies and minimize their effects on the output of the model.

Essentially, sensitivity analysis involves the perturbation of individual input variables over a wide range of realistic values, yielding variations in output. The resulting variation in output, as a function of the input variables, is compared with the real world to ensure that the output is what is expected, taking into consideration the assumptions inherent to the model. Initially, only one input variable at a time should be varied, and the others should be held constant. Then, if time, resources, and complexity of the model warrant, combinations of variables can be varied simultaneously.

Another function of sensitivity analysis is to determine the input variables to which the model is most sensitive. The implication from such an analysis would be that the more sensitive the model is to a given input, the more effort should be expended to obtain the most correct or representative value for that input.

CALINE2 is a fairly straightforward model in terms of the interactions of the input variables. The sensitivity analysis performed on CALINE2 is, therefore, more of an exercise to demonstrate that the output behaves as one would intuitively expect from the form of the equations. As a model becomes more complex and less intuitively obvious, a properly conducted sensitivity analysis becomes more necessary.

Sensitivity to Source Strength

The source strength terms in CALINE2 consist of the traffic volume VPH, the average emission factor EF, and, for parallel winds only, the highway width W. Since these terms are in the numerators of the line source equations (equations 2, 3, and 5), the calculated pollutant concentrations are directly proportional to them, and the resulting sensitivities are linear. Figures 15 and 16 show that, for a given change in either VPH or EF, the predicted CO changes correspondingly. In other words, if either VPH or EF is doubled, the predicted CO is doubled.

Figure 17 shows that the highway width has an inverse effect on the predicted CO, i.e., as W increases, CO decreases. This effect occurs because W is not only incorporated into the source strength term for parallel winds, but is also used to modify the initial segment of the σ_z curve as discussed in an earlier section. It appears reasonable that, as the volume of air in the mixing cell increases, while the VPH and EF remain the same, the predicted CO concentration should decrease.

Only the predicted CO concentrations in the mixing cell are shown for only 1 wind angle, an at-grade highway, and 1 stability class. For most of the CALINE2 sensitivities, the sensitivity in the mixing cell (for a given wind angle and so on) will be similar to the sensitivity at a receptor away from the highway (and for different wind angles and so on). In the cases where it is not, sensitivities at separate removed receptors (or different wind angles and so on or both) are shown.

Sensitivity to Wind Speed

CALINE2 sensitivity to wind speed is shown in Figure 18. The hyperbolic increase in predicted CO levels as wind speed decreases is clearly shown. The limit of the model of 3.2 km/h or 2 mph is indicated by the dashed line. Both cross and parallel wind mixing cells are displayed, and one can see the similarity between the two.

Sensitivity to Wind Angle

Figure 19 is the sensitivity of the concentration of the mixing cell to changes in the angle of the wind for all stability classes. All stability classes have the same mixing cell concentration for an exactly perpendicular (ϕ = 90 deg) wind, and they have the greatest difference for an exactly parallel (ϕ = 0 deg) wind. Obviously, since stability class F is the most stable, the most parallel wind buildup in the mixing cell will occur with this class, and this is what Figure 19 shows. On the other hand, stability class F will confine the pollutants near the highway under parallel winds because of very little turbulence to spread the plume. For stability class A the large degree of turbulence will spread the plume away from the highway. Figure 20 shows this situation for a receptor 120 m away from the highway at ground level. In this case, a 90-deg wind yields the greatest spread in concentrations, as a function of stability class, since the wind is blowing directly toward the receptor, with the most stable air causing the highest pollutant level at the receptor. The scale of predicted CO shown in Figure 19 is greatly reduced from that shown in Figure 20. The uncertainty of the quality of the input and the Gaussian assumptions result in estimates that are at best accurate to the nearest part per million (or microgram per cubic meter) and not to a tenth of that unit. Therefore, the concentrations shown are in reality all the same and are close to ambient. However, for the sensitivity analysis, the calculated values are used to demonstrate the relative importance of input variables.

Sensitivity to Pavement Height

CALINE2 sensitivity to pavement height is a more difficult analysis to make. The definition of the mixing cell determines that the concentration within the mixing cell will be the same regardless of where the highway is in relation to the surrounding terrain. Thus, the sensitivity for the input parameter of pavement height is shown in Figure 21 for a receptor that is parallel to the edge of the mixing cell but at ground level. This implies that the receptor will be above the highway for a depressed section (negative pavement height) and below the highway for a raised section (positive pavement height). As expected, the predicted CO concentration for this receptor decreases as the highway is either lowered or raised from grade. Parallel winds cause the decrease to be larger.

Sensitivity to Stability Class

The definition of the mixing cell used in CALINE2 implies its concentration is independent of surface atmospheric stability. This is shown in Figure 22 for crosswinds. For parallel winds, an exponential increase in concentrations is evidenced as stability increases because of the buildup.

Figure 16. CALINE2 sensitivity to emission factor.

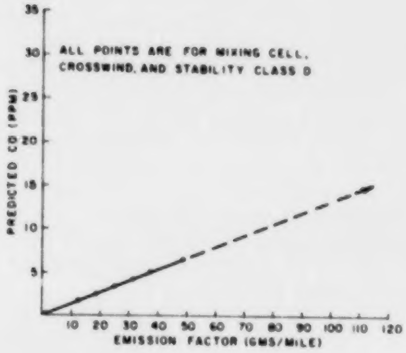


Figure 17. CALINE2 sensitivity to highway width.

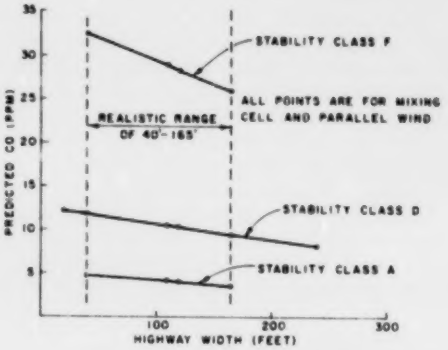


Figure 18. CALINE2 sensitivity to wind speed.

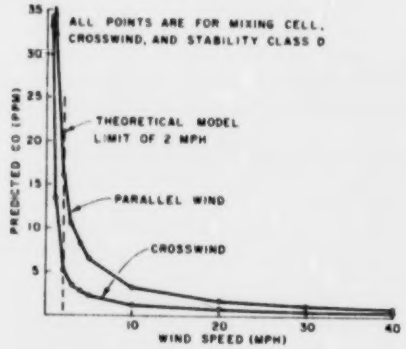


Figure 19. CALINE2 sensitivity to wind angle and mixing cell concentration.

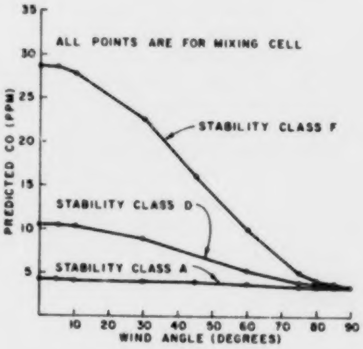


Figure 20. CALINE2 sensitivity to wind angle and off-highway concentration.

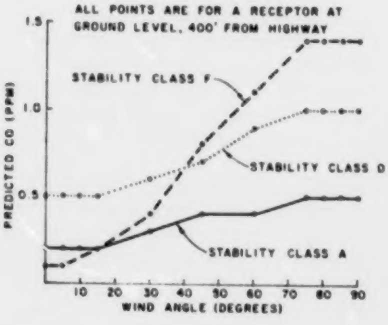
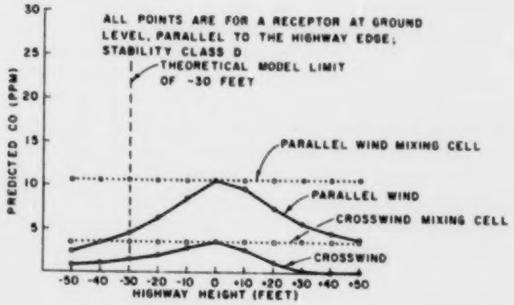


Figure 21. CALINE2 sensitivity to pavement height.



Ranking of Sensitive Parameters

From the preceeding sensitivity analysis, the following general ranking can be placed on the input variables. CALINE2 is most sensitive to the wind vector because it affects a number of inputs to the model. The direction of the wind vector in relation to the highway is important since angles approaching 0 deg cause parallel wind buildup. Stability class is a function of wind speed and is a fairly sensitive input, since F stability confines pollutants and A allows substantial dispersion. Wind speed itself is important because the calculated concentrations are inversely proportional to it, which means that a halving of the wind speed would cause a doubling of the predicted concentration. The source strength terms of VPH and EF are as sensitive as the wind vector, although they do not have a multiple influence on the model. The predicted concentrations are a direct function of VPH and EF, and a change in either term causes a corresponding change in the output. Pavement height and highway width are important parameters, but are relatively less important to CALINE2 than any other input.

PRELIMINARY VERIFICATION

Interpretation of Results

The California Department of Transportation is under contract with the Federal Highway Administration to provide an aerometric data base for the purpose of verifying and calibrating line source models (10). As part of this work, a preliminary data base for hourly averages of carbon monoxide concentrations was obtained by using bag sampling procedures in the Los Angeles area in 1972 (7). Three types of highway geometrics were monitored, including 2 depressed sections, 1 at-grade section, and 1 fill section. Figure 23 shows the locations of the sites.

Measurements for this study at any 1 site consisted of as many as 24 carbon monoxide sampling points for the integrated 1-hour CO concentrations, 1-hour values of surface wind speeds and directions, and 1-hour traffic counts. This last information and the highway configuration were used as input to CALINE2 to produce simulations that were then compared with the measured CO concentrations. The comparisons were used to determine the predictive capabilities of the model.

Linear regression analysis was used to compare the scatter plot of observed CO concentrations versus predicted CO concentrations. The figures referred to in this section that show the preliminary verification results contain the regression information for each comparison. This information includes the regression line, the regression equation, the sample size n, the standard error of the estimate, the correlation coefficient r, and the F-test value for a 5 percent level of significance.

The regression line shows how well the model predicts in comparison with measured concentrations. If the line slope is less than 1, the model overpredicts. If the line slope is greater than 1, the model underpredicts. If the line is coincident with the 45-deg line, the model is making nearly perfect predictions, depending on the values of the other regression parameters. Since the model calculates downwind concentrations from the line source only (i.e., above ambient), the upwind (ambient) level was subtracted from the measured mixing cell and downwind concentrations before a comparison was made to the simulated values.

The verifications are separated into highway configurations (at-grade, depressed, and fill), wind angles (cross and parallel), and on- and off-highway sites to better determine how each of these situations can be handled by CALINE2. Obviously, some of the verifications are questionable because of the small sample size; however, they were included to give a relative indication of CALINE2 capabilities. Larger sample sizes could have been obtained by combining all sites and situations, but this would have resulted in data gaps and thereby obscured the predictive characteristics of the model for each individual situation.

For instance, the mixing cell generally has higher concentrations than off-highway points have. When plotted together, the mixing cell points may form a cluster away from the origin, while the off-highway points may cluster close to the origin, leaving a gap between the 2 clusters. A regression analysis would indicate that there is a good regression between these 2 clusters, but would not indicate the correlation within each cluster. Therefore, the clusters are broken into separate categories, as in this analysis.

For all of the regressions, all stability classes have been combined, because there were insufficient data pairs to separate the analyses by stability. The predominant stability classes encountered were those for unstable through neutral surface atmospheric conditions, i.e., classes A through D. Only a few cases had stabilities of E or F. Therefore, it is difficult to draw any conclusions about the ability of CALINE2 to handle stable and very stable atmospheric conditions. A more extensive verification of CALINE2 is planned in which data recently gathered in the Los Angeles area will be used with the transportation department's mobile air quality vans (10). At that time, the analysis will be separated into as many verification categories as possible, including stability classes.

At-Grade Site

The at-grade site was located at the weigh station on the San Diego Freeway, just southeast of the junction with the Harbor Freeway. Figure 24, a schematic of the site, shows how the probes were placed for the prevailing west wind. Probe 3 was designed to be used as the upwind sampling intake. Probes 6 and 9 were averaged by using weighted factors derived from the traffic flow in each direction to obtain the "measured" mixing cell concentration.

Figures 25, 26, and 27 show the crosswind situation for the at-grade site and show that CALINE2 overpredicts by a factor of 2 for the mixing cell points, does fairly well for off-highway sites, and yields a reasonable correlation for the combined plots. The parallel wind (Figures 28, 29, and 30) sampling sizes are much smaller, but generally show that CALINE2 is able to handle parallel wind situations reasonably well.

The regression for the crosswind and mixing cell may indicate a falsely high overprediction because of the manner in which the measured mixing cell concentrations were obtained. The concentration at probe 6 tended to be much lower than that at probe 9 under moderate wind speeds, thereby disagreeing with the assumption that a uniform mixing cell exists across the width of the highway. Simulations for each traffic direction might yield better correlations, but this task has yet to be undertaken.

Depressed Sites

The depressed sites were at the Fourth Avenue pedestrian overcrossing of the Santa Monica Freeway and the Harbor Freeway at 146th Street. These were true depressed sites, being depressed from the surrounding terrain for noise control or other purposes, and not simple cuts into the sides of hills. Figure 31 is a schematic of the Santa Monica site. The probes are equally distributed on either side of the site because parallel winds were anticipated and it was necessary to maintain maximum flexibility for downwind probe sites. Probes 10 and 11 were averaged to obtain the mixing cell concentration for this site. Figure 32 is the schematic of the Harbor Freeway site; probes 3 and 4 were designed to be used as the upwind intakes. Probes 6 to 10 were averaged via weighted factors in the same manner as the at-grade site to obtain the measured mixing cell concentrations.

Figures 33 through 38 show that CALINE2 appears to be able to handle the depressed section situation quite well, with a slight overprediction. However, one must remember that data from these same sites were used to develop the depressed section ratios discussed earlier. Full verification of the model for this situation must wait until the CO data are available from the department's research project (10).

Figure 22. CALINE2 sensitivity to stability class.

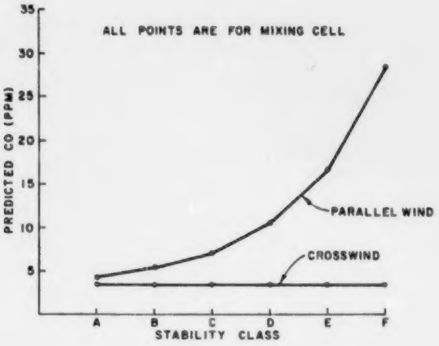


Figure 23. Los Angeles sampling project.

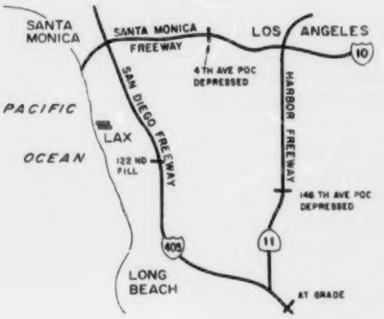

SANTA MONICA
SANTA MONICA FREEWAY
LOS ANGELES
10
4 TH AVE POC DEPRESSED
SAN DIEGO FREEWAY
HARBOR FREEWAY
PACIFIC
OCEAN
LAX
122 ND FILL
146 TH AVE POC DEPRESSED
405
11
LONG BEACH
AT GRADE

Figure 24. Probe locations at weigh station on San Diego Freeway.

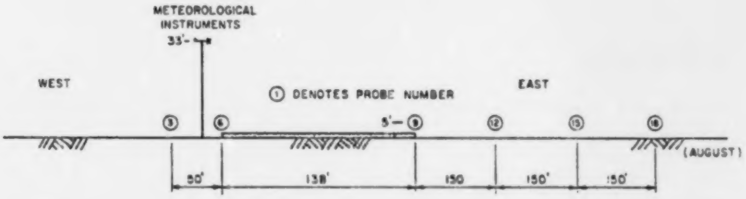

METEOROLOGICAL INSTRUMENTS
33'
WEST
EAST
① DENOTES PROBE NUMBER
③
⑥
5'
⑨
⑫
⑮
⑱
(AUGUST)
50'
138'
150
150'
150'

Figure 25. At-grade site, crosswind, and mixing cell points.

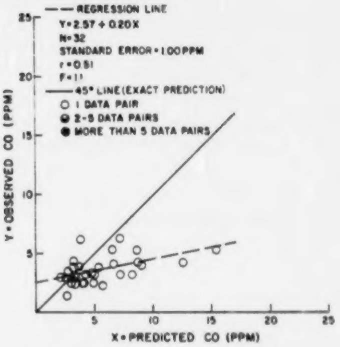


Figure 26. At-grade site, crosswind, and off-highway ground-level points.

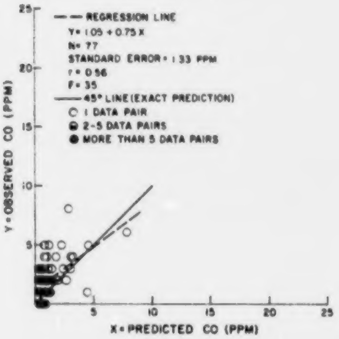


Figure 27. At-grade site, crosswind, and off-highway ground-level and mixing cell points.

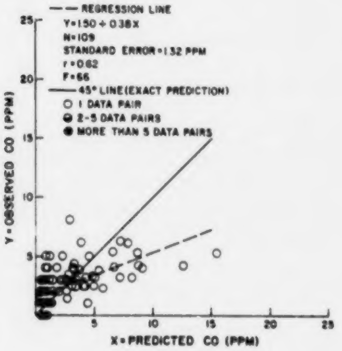


Figure 28. At-grade site, parallel wind, and mixing cell points.

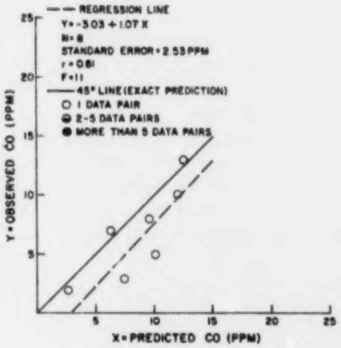


Figure 29. At-grade site, parallel wind, and off-highway ground-level points.

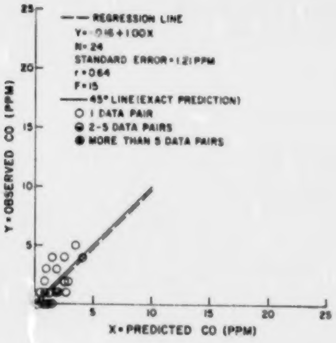


Figure 30. At-grade site, parallel wind, and off-highway ground-level and mixing cell points.

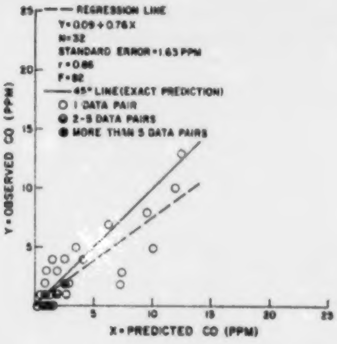


Figure 31. Probe locations at Santa Monica Freeway at Fourth Avenue.

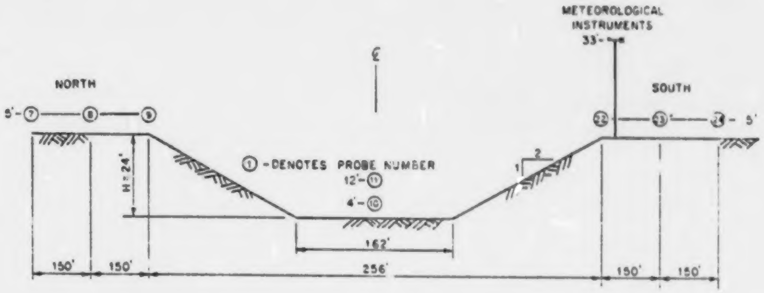

METEOROLOGICAL INSTRUMENTS
33'
℄
NORTH
SOUTH
5'-⑦
⑧
⑨
㉒
㉓
㉔- 5'
H=24'
① -DENOTES PROBE NUMBER
12'-⑪
4'-⑩
1
2
162'
150'
150'
256'
150'
150'

Figure 32. Probe locations at Harbor Freeway at 146th Street.

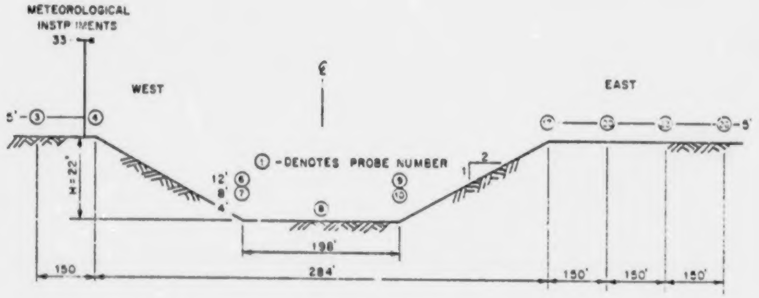

METEOROLOGICAL INSTRUMENTS
33
℄
WEST
EAST
5'-③
④
H=22'
① -DENOTES PROBE NUMBER
12' ⑥
8' ⑦
4'
⑧
⑨
⑩
1
2
-5'
198'
150
284'
150'
150'
150'

Figure 33. Depressed sites, crosswind, and mixing cell points.

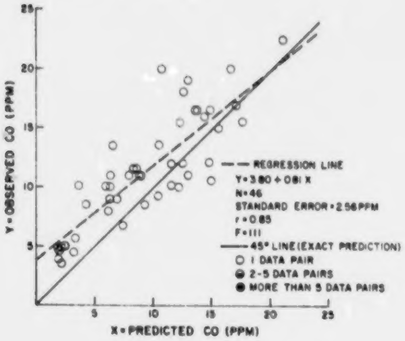


Figure 34. Depressed sites, crosswind, and off-highway ground-level points.

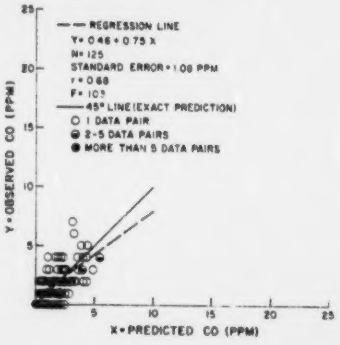


Figure 35. Depressed sites, crosswind, and off-highway ground-level and mixing cell points.

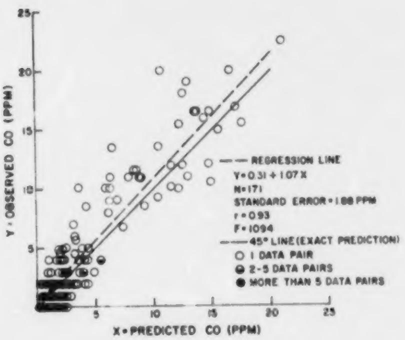


Figure 36. Depressed sites, parallel wind, and mixing cell points.

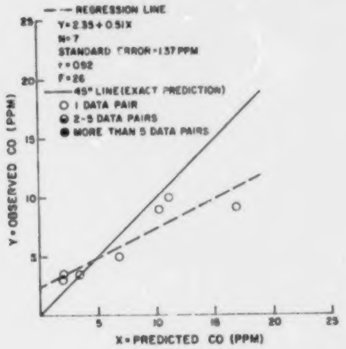


Figure 37. Depressed sites, parallel wind, and off-highway ground-level points.

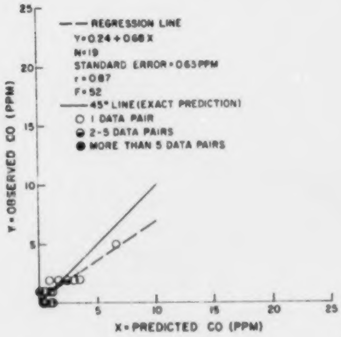


Figure 38. Depressed sites, parallel wind, and off-highway ground-level and mixing cell points.

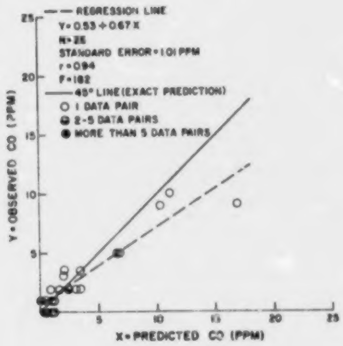
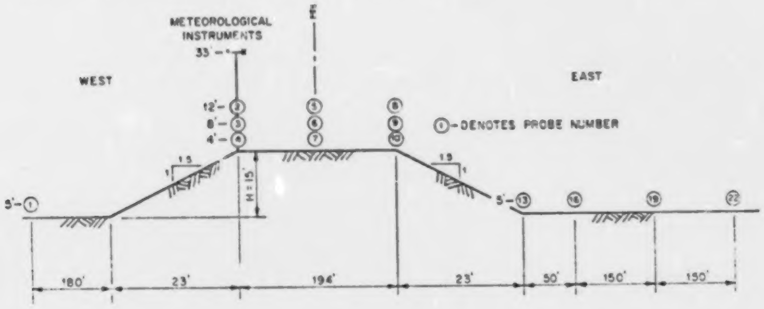


Figure 39. Probe locations at San Diego Freeway at 122nd Street.


METEOROLOGICAL INSTRUMENTS
33'
WEST
EAST
12'
8'
4'
2
3
4
5
6
7
8
9
10
1 - DENOTES PROBE NUMBER
1.5
1
H = 15'
5'
1
5'
13
16
19
22
180'
23'
194'
23'
50'
150'
150'

Fill Site

The fill site was on the San Diego Freeway at 122nd Street and is shown schematically in Figure 39. Probe 1 was obviously the upwind probe, and probes 2 to 10 were averaged in the same manner as the other sites to obtain the measured mixing cell concentrations.

Figures 40, 41, and 42 show how CALINE2 overpredicts the concentrations resulting from a fill section for a crosswind. There was no parallel wind data for this site. As for the at-grade site, the overprediction factor of 2 for the mixing cell could be a false comparison, for the concentrations for the upwind probes on the edge of the highway (probes 2 to 4) tended to be much lower than those for the probes on the downwind edge (probes 8 to 10).

APPLICATIONS

Overall Use of CALINE2

CALINE2 should be used to determine the air quality impact of a proposed highway or other relatively constant linear source of air pollutants. Although CALINE2 only calculates the estimated dispersion of carbon monoxide from a line source, this dispersion will give an indication of the atmospheric movement of other pollutants, such as lead and sulfate particulates, nitric oxides, and hydrocarbons. (This assumes that the particulates can be characterized in their transport and diffusion as gases and that there are no chemical reactions of the other pollutants.) The model cannot, in its present form, be used to calculate the resultant concentrations of these other pollutants because of the gravitational settling of particulates and chemical reactions. It can, however, yield hourly average CO estimates that are slightly on the conservative side of actual CO concentrations for most cases as long as the constraints and assumptions of the model are observed.

CALINE2 can be used in the design process of a proposed line source (highway) to determine which configurations would result in the smallest CO concentrations for the given meteorology of a site. An analysis can be made of alternative sites (along with alternative configurations) to determine which meteorology will disperse the pollutant load most adequately.

Most proposed line source projects will be more than a simple straight line maintaining a constant angle to the prevailing winds and at the same height above or below grade. CALINE2 has no internal capability of superposition that would allow the calculation of pollutant contributions from different configurations of sections, but the contribution of each section can be simulated on a separate run of the model and then summed later either by hand or by another computer program. When the proposed project involves a number of short varying segments (shorter than 1.6 km in length), or complex situations, such as cloverleaf interchanges, other assumptions and simplifications will have to be made about the configurations of the project before CALINE2 is used. These simplifications will result in a greater departure from the real-world situation, but the estimated dispersions should still give an approximate idea of the actual dispersion.

Of course, other environmental design considerations will have to be taken into account in the decision reached on the line source configuration. Environmental siting of a line source should not be based on air quality impact alone.

CALINE2 Simulations

Figure 43 shows the flow of information into the model, the calculations made in model, and the resulting output. The output can be in micrograms per cubic meter or parts per million. Figure 44 shows a printout of the carbon monoxide concentrations in parts per million as calculated by CALINE2 for a crosswind, oblique wind, and parallel wind.

Figure 40. Fill site, crosswind, and mixing cell points.

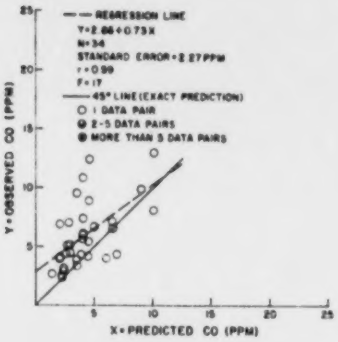


Figure 42. Fill site, crosswind, and off-highway ground-level and mixing cell points.

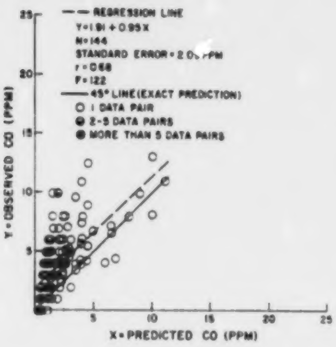


Figure 43. Flow chart for CALINE2 model.

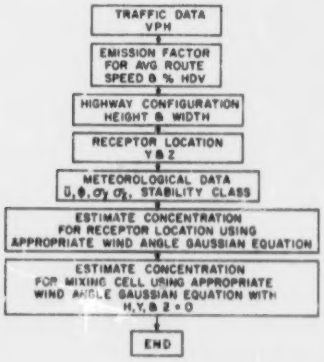

TRAFFIC DATA VPH
EMISSION FACTOR FOR AVG ROUTE SPEED & % HDV
HIGHWAY CONFIGURATION HEIGHT & WIDTH
RECEPTOR LOCATION Y & Z
METEOROLOGICAL DATA $\bar{u}, \phi, \sigma_y, \sigma_z$, STABILITY CLASS
ESTIMATE CONCENTRATION FOR RECEPTOR LOCATION USING APPROPRIATE WIND ANGLE GAUSSIAN EQUATION
ESTIMATE CONCENTRATION FOR MIXING CELL USING APPROPRIATE WIND ANGLE GAUSSIAN EQUATION WITH H, Y, & Z = 0
END

Figure 41. Fill site, crosswind, and off-highway ground-level points.

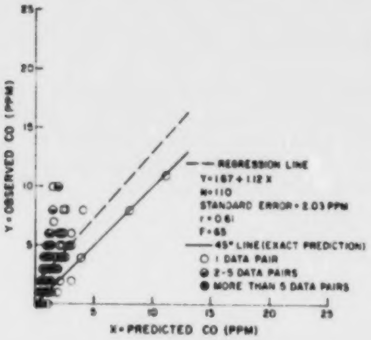
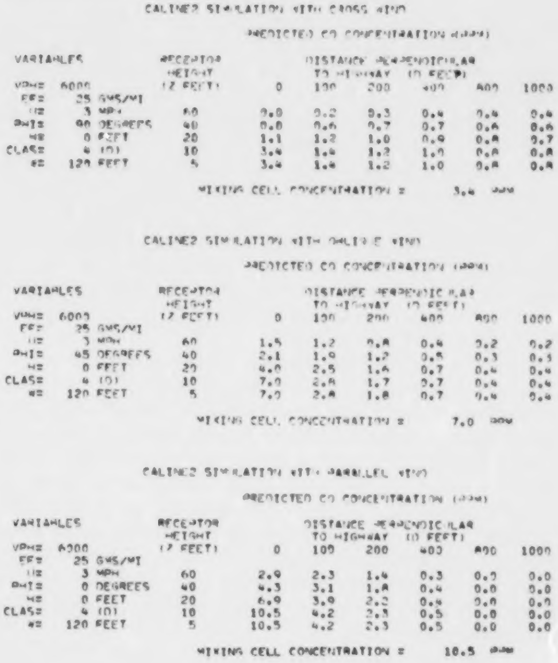


Figure 44. Printout of CALINE2 simulations.



```
                   CALINE2 SIMULATION WITH CROSS WIND

                          PREDICTED CO CONCENTRATION (PPM)

  VARIABLES          RECEPTOR             DISTANCE PERPENDICULAR
                      HEIGHT              TO HIGHWAY   (D FEET)
  VPH=  6000         (Z FEET)       0      100     200     400     800    1000
   EF=    25 GMS/MI
    U=     3 MPH         60        0.0     0.2     0.3     0.4     0.4     0.4
  PHI=    90 DEGREES     40        0.0     0.6     0.7     0.7     0.6     0.6
    H=     0 FEET        20        1.1     1.2     1.0     0.9     0.8     0.7
 CLASS=    4 (D)         10        3.4     1.4     1.2     1.0     0.8     0.8
    W=   120 FEET         5        3.4     1.4     1.2     1.0     0.8     0.8

                    MIXING CELL CONCENTRATION =        3.4  PPM


                   CALINE2 SIMULATION WITH OBLIQUE WIND

                          PREDICTED CO CONCENTRATION (PPM)

  VARIABLES          RECEPTOR             DISTANCE PERPENDICULAR
                      HEIGHT              TO HIGHWAY   (D FEET)
  VPH=  6000         (Z FEET)       0      100     200     400     800    1000
   EF=    25 GMS/MI
    U=     3 MPH         60        1.5     1.2     0.8     0.4     0.2     0.2
  PHI=    45 DEGREES     40        2.1     1.9     1.2     0.5     0.3     0.3
    H=     0 FEET        20        4.0     2.5     1.6     0.7     0.4     0.4
 CLASS=    4 (D)         10        7.0     2.8     1.7     0.7     0.4     0.4
    W=   120 FEET         5        7.0     2.8     1.8     0.7     0.4     0.4

                    MIXING CELL CONCENTRATION =        7.0  PPM


                   CALINE2 SIMULATION WITH PARALLEL WIND

                          PREDICTED CO CONCENTRATION (PPM)

  VARIABLES          RECEPTOR             DISTANCE PERPENDICULAR
                      HEIGHT              TO HIGHWAY   (D FEET)
  VPH=  6000         (Z FEET)       0      100     200     400     800    1000
   EF=    25 GMS/MI
    U=     3 MPH         60        2.9     2.3     1.4     0.3     0.0     0.0
  PHI=     0 DEGREES     40        4.3     3.1     1.8     0.4     0.0     0.0
    H=     0 FEET        20        6.9     3.9     2.2     0.4     0.0     0.0
 CLASS=    4 (D)         10       10.5     4.2     2.3     0.5     0.0     0.0
    W=   120 FEET         5       10.5     4.2     2.3     0.5     0.0     0.0

                    MIXING CELL CONCENTRATION =       10.5  PPM
```

Cost and Availability

CALINE2 requires minimal computer time for simulation runs, especially when used on the large digital computers. On the IBM 370/168, a typical computer run of 42 separate line source simulations (with 36 receptor sites per simulation) requires 11.5 CPU seconds at an approximate cost of $3. Generally, therefore, CALINE2 represents a relatively cheap, fast method to obtain reasonable estimates of CO concentrations for a future highway or other line source.

CALINE2 is currently programmed in FORTRAN on the California IBM system 370/168 and in BASIC on the Department of Transportation's TENET time-sharing facility. A computer listing and source deck of the program as written in FORTRAN IV-G for the IBM 370/168 can be obtained at a nominal cost by public agencies on request to the California Department of Transportation. With the approval of the Federal Highway Administration, the same information can be released to private enterprises.

Future Work

CALINE2 does not yet represent a polished end product, merely an interim tool that can be used by transportation planners to obtain estimates of impacts of highways on local air quality. Work remaining to be done includes the following:

1. Fine-tuning calibration and verification with extensive field sampling data that are becoming available (10);
2. Development of a grid or superposition version of the model that will allow the analysis of multiple line sources and modal systems;
3. Evaluation of a possible modification of the model to estimate dispersion of lead and sulfate particulates; and
4. Comparison of predictive capabilities of CALINE2 with those of other line source models, such as HIWAY of the U.S. Environmental Protection Agency.

The state of the art for air pollution modeling is rapidly changing, and attempts will be made to keep CALINE at the forefront of those changes.

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3. W. A. Carpenter and G. G. Clemeña. The Theory and Mathematical Development of AIRPOL-4. Virginia Highway and Transportation Research Council, Publ. VHTRC 75-R49, May 1975.
4. F. L. Ludwig and W. F. Dabberdt. Evaluation of the APRAC-1A Urban Diffusion Model for Carbon Monoxide. Stanford Research Institute, Menlo Park, Calif., 1972.
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10. Air Pollution and Roadway Location, Design, and Operation. Transportation Laboratory, California Department of Transportation.
11. M. D. Batham. Air Quality Manual Modification Number 3: Revision of Existing Emission Factors Based Upon EPA Manual AP-42. Transportation Laboratory, California Department of Transportation, Sept. 1974.

MICROSCALE MODELING OF NEAR-ROADWAY AIR QUALITY BY NUMERICAL TECHNIQUES

John Sontowski, Bureau of Technical Services, New York City Department of Air Resources

The type of microscale modeling considered here is that based on the numerical solution of partial differential equations that govern the conservation of pollutant species throughout specified regions of the atmosphere. The regions considered are small, generally including a roadway and nearby points at distances of tens or hundreds of meters. Thus the use of the term microscale.

Figure 1 shows a schematic diagram of the modeling approach under consideration. The arrows represent processes leading to products shown in boxes. A pollutant species within any selected volume of the atmosphere is conserved by a balance of transport into and out of the volume, production (or depletion) by chemical reactions, and other internal sources or sinks. Mathematically this can be specified by requiring that, for any given species at any time within a volume about a general point x, y, z,

Rate of increase = rate transported in - rate transported out
+ net rate of chemical production
+ net rate of production from internal sources and sinks

By considering the limit as the volume becomes infinitesimally small, this conservation can be expressed in the form of a governing partial differential equation:

$$\frac{\partial x}{\partial t} = -u\frac{\partial x}{\partial x} - v\frac{\partial x}{\partial y} - w\frac{\partial x}{\partial z} + \frac{\partial}{\partial x}\left(K_x\frac{\partial x}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial x}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial x}{\partial z}\right)$$

$$+ R_c + R_s$$

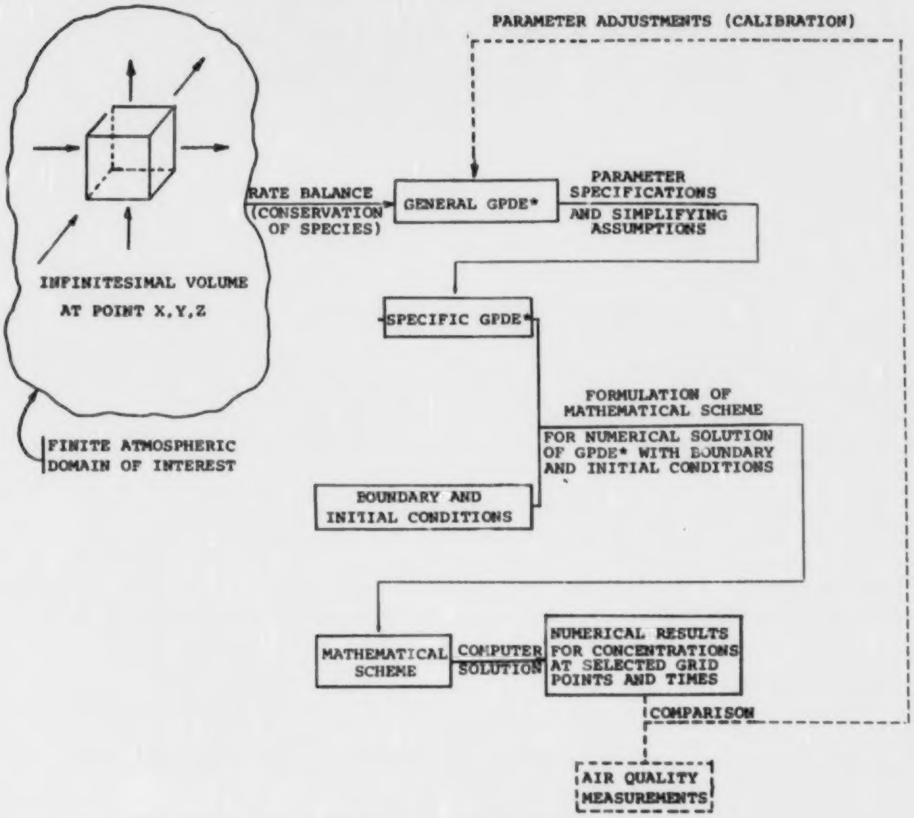
where

x = concentration;
u,v,w = mean wind velocity components in x, y, z directions respectively;
K_x,K_y,K_z = turbulent diffusion coefficients in x, y, z directions respectively;
R_c = net rate of chemical production per unit volume; and
R_s = net rate of production per unit volume from sources and sinks.

The above equation was developed with a coordinate system fixed in space (Eulerian formulation). An alternative but equivalent form is sometimes developed with a coordinate system moving with the atmosphere (Lagrangian formulation).

The first 3 terms on the right side of the equation represent net transport in the

Figure 1. Schematic diagram of microscale model.


PARAMETER ADJUSTMENTS (CALIBRATION)
INFINITESIMAL VOLUME
AT POINT X,Y,Z
FINITE ATMOSPHERIC
DOMAIN OF INTEREST
RATE BALANCE
(CONSERVATION
OF SPECIES)
GENERAL GPDE*
PARAMETER
SPECIFICATIONS
AND SIMPLIFYING
ASSUMPTIONS
SPECIFIC GPDE*
FORMULATION OF
MATHEMATICAL SCHEME
FOR NUMERICAL SOLUTION
OF GPDE* WITH BOUNDARY
AND INITIAL CONDITIONS
BOUNDARY AND
INITIAL CONDITIONS
MATHEMATICAL
SCHEME
COMPUTER
SOLUTION
NUMERICAL RESULTS
FOR CONCENTRATIONS
AT SELECTED GRID
POINTS AND TIMES
COMPARISON
AIR QUALITY
MEASUREMENTS

*GPDE: GOVERNING PARTIAL DIFFERENTIAL EQUATION TO BE SATISFIED AT EACH TIME T AND EACH POINT X, Y, Z WITHIN ATMOSPHERIC DOMAIN OF INTEREST. (NOT A SOLUTION OR EXPLICIT EQUATION FOR POLLUTANT CONCENTRATION)

various directions by the mean wind components; the second 3 terms represent the transport by the turbulent components, i.e., by turbulent diffusion. Molecular diffusion is negligible in comparison and thus does not appear. An equation of this form applies to each pollutant, except that the chemical reaction and source production terms (R_c and R_s) are different. The chemical reaction term complicates the analysis considerably because it involves not only the particular pollutant of interest but all others with which it reacts. Thus, the governing equation is coupled to similar equations for other pollutants, making it necessary to solve simultaneously a set of partial differential equations. However, carbon monoxide for microscale purposes is essentially an inert species, and therefore the chemical reaction term will be neglected. Thus, we need to solve only a single, uncoupled, partial differential equation. The resulting equation is the general governing partial differential equation (GPDE) referred to in Figure 1. The word general should be qualified since the equation has a specific form that treats turbulent transport as a function proportional to the gradient of concentration. The coefficients of proportionality are the turbulent diffusion coefficients K_x, K_y, K_z. This form of the equation is used because it is the classical and most common formulation and the one used in the models being considered.

It may be helpful to point out that modeling of the type considered here is frequently described in the air pollution literature by the terms K-theory and conservation of mass. The K-theory designation is attributable to the use of the symbol K as the turbulent diffusion coefficient. Conservation of mass refers to the governing partial differential equation and its derivation based on the conservation of a particular species of pollution. This term may be somewhat confusing to those familiar with the literature on fluid dynamics and transport phenomena. In these sciences, conservation of mass generally refers to the equation for conservation of the total mass made up of the sum of the masses of all species. The equation for an individual species, such as that being treated here, is then referred to as the conservation of species equation, or some similar terminology.

The modeling approach shown in Figure 1 proceeds by specifying the spatial and temporal distribution of parameters (such as u, K_x, and R_s) and by making simplifying assumptions, thus reducing the general GPDE to a specific form applicable to a particular problem of interest. The coefficients u, v, w, K_x, K_y, and K_z can be specified on the basis of micrometeorological data, empirical profiles, fluid dynamics, and turbulence theory or by solving partial differential equations for u, v, and w based on conservation of mass, momentum, and energy. The emission rate R_s is of course based on a source inventory involving traffic data with emission factor analysis (25). Simplifying assumptions can involve neglecting terms of the GPDE or using simplified forms of the coefficient terms u, v, w, K_x, K_y, and K_z. Bases for neglecting terms completely include boundary layer theory, steady state, and dimensional homogeneity or uniformity, e.g., neglecting the direction parallel to a long, uniform highway line source. The resulting specific GPDE must then be satisfied at every point in the atmospheric domain of interest. To complete the mathematical formulation of the problem, however, requires that conditions be specified on the boundaries of the atmospheric domain (boundary conditions) and at some initial time throughout the domain (initial conditions). These conditions are given in terms of either the concentration or the concentration gradient or a combination of both. Physically such conditions are related to either the pollutant flux or the pollutant concentration, which in turn can be related to emission rates and background, measured, or other known concentrations. Frequently all sources can be accounted for at the boundaries, thus eliminating the internal source term R_s from the GPDE.

The above boundary and initial conditions together with the specific GPDE constitute the mathematical differential statement of the specific problem of interest. Solution of such problems can be achieved, or attempted, by any of a number of methods including techniques for exact solution leading to analytical expressions (explicit or implicit algebraic-transcendental equations for concentration), techniques for approximate solution leading to analytical expressions, or numerical techniques leading directly to numerical results at an array of grid points and at specific times. Our present consideration is directed toward the last approach, i.e., numerical techniques. The Gaussian equation, on the other hand, is an exact solution to a highly simplified GPDE.

The use of numerical techniques involves the formulation of some mathematical scheme for the calculation of numerical results that will satisfy the specific GPDE with its associated boundary and initial conditions. The mathematical scheme is then computerized for calculation of the results. In most cases the numerical technique used is the finite difference approach. Most cases, however, differ from one another by application of different variations of the finite difference approach. Although these variations do not change the basic objective of satisfying the GPDE with associated conditions, they can have an effect on the accuracy of doing so and, probably more significant, they can have considerable impact on computation efficiency and therefore on computer requirements.

This discussion covers all ingredients essential to description of our modeling approach. Figure 1, however, also shows how the approach can be improved, and usually is, by comparison with air quality data and calibration through adjustment of the coefficient parameters.

EXISTING NUMERICAL MODELS: STATE OF THE ART

Following is a brief description of existing capabilities and some specific models (1, 2, 3, 4, 5, 6, 7, 8, 9, 10) based on numerical techniques. The list of models is not all inclusive, but is representative of the various degrees and avenues of development. Figure 1 shows the primary elements that distinguish models: atmospheric domain, boundary conditions, parameter specifications and simplifying assumptions, and mathematical scheme. Although these factors determine the capabilities of models, a definitive evaluation should also consider the degree and success of model validations. Unfortunately, validations have not been performed for all models, and those that have been performed are not adequate for evaluation of the relative merits of models. Along these lines it would be helpful if all modelers evaluated a common set of validation criteria, such as correlation coefficients and standard error of estimate.

Atmospheric domain and boundary conditions essentially determine the problem that is solved; parameters and assumptions determine the limitations and rigor with which it is solved, and the mathematical scheme determines the computational efficiency. The problems most commonly solved by existing models involve elevated, at-grade, and depressed roadways. In addition, however, there are models of complexity sufficient to deal with 3-dimensional multiroadway systems in the presence of complex building and topographical features.

Specifications for wind and turbulence parameters include analytical profiles such as power and logarithmic laws, separated flow regions with backflow and vortex motions in the vicinity of obstructions, and, in the most sophisticated cases, flows determined by solution of the partial differential equations governing conservation of mass and momentum. Although each existing model has been applied with only selected wind and turbulence profiles, all the models have the mathematical capability, and are generally programmed on the computer, to accept any prescribed profiles. However, one qualification that is usually built into the program, or should be, is the constraint that winds must be such as to conserve total mass at all points of the atmospheric domain; i.e., they must satisfy the partial differential equation for conservation of mass (total mass). In this way the models prevent impossible flow fields that artificially create or destroy atmospheric mass, including mass of the particular species of interest. With the flexibility of accepting arbitrary wind and turbulence input, models may be readily upgraded as more accurate information, data, or analysis becomes available for each input.

Regarding the simplifying assumptions, most models assume 2-dimensional steady-state behavior, although some include 3-dimensional and transient effects. The 2-dimensional assumption is applicable to long roadways with uniform topography and emissions along their length. Except near the ends of such roadway sections, variations parallel to the road are negligible.

Details of the mathematical scheme employed are quite complex and diverse and are thus difficult to evaluate except on the basis of their effect on the relative computational efficiency of the various models. The efficiencies in terms of computer requirements such as running time and storage have been surveyed and reported by Darling (11) for numerous models including both numerical and Gaussian types. An updated version including additional models would be valuable and should be available in the near future.

Egan and Lavery (1) treat elevated, at-grade, and depressed roadways and also include applications to at-grade and elevated roadways upwind of an obstacle. The model is 2-dimensional steady-state with perpendicular or near-perpendicular winds. Validations have been performed for vertical power law wind and turbulence profiles with eddy recirculation regions in the vicinity of obstacles.

The General Research Corporation (GRC) model (2) incorporates several unique features. The mathematics is composed of a hybrid of finite differences in the vertical, the Gaussian distribution in the cross-wind direction, and a Lagrangian formulation for the windward transport. As a result the model is capable of handling 3-dimensional time-dependent problems of arbitrary wind direction with greatly reduced computer requirements. The model also takes advantage of advanced aerodynamics to simulate wake velocity and turbulence distributions both behind vehicles and downwind of elevated roadways (open underneath). Unfortunately the model has not been validated.

Elevated roadways are of 2 basic types: those that are filled underneath and those that are open underneath. The aerodynamics of the 2 cases, and therefore the resulting concentration fields, are considerably different. Thus, a model derived and calibrated for one type should not be expected to give good results for the other. Similarly, caution should be exercised in the application of models for depressed roads, since the depressions modeled can be quite different, ranging from shallow to deep, with vertical or sloping walls and with other irregularities such as cantilevered overhands.

Kirsch and Mason (3) describe a model known as EXPLOR. It allows arbitrary wind direction and has been validated for elevated, at-grade, and depressed roadways. Effects of irregular terrain are accounted for by constructing a wind field that satisfies the equation for conservation of total mass. A related model is called NEXUS (4). This is essentially a 3-dimensional version of EXPLOR. Recently EXPLOR and NEXUS have been upgraded, primarily by incorporation of a subprogram called W-FIT, which determines an improved wind distribution by solving the governing partial differential equations for conservation of momentum of an inviscid fluid. In addition, the models have been expanded to allow more than 1 roadway, currently as many as 8, with arbitrary vertical and horizontal spacing. The new NEXUS is particularly suited for treatment of 3-dimensional stacked roadway configurations as found in typical interchanges. The upgraded versions of NEXUS and EXPLOR are called MROAD 2 and MROAD 3 respectively. Draft copies of user manuals for the new programs have been provided, under contract, to the Oregon Department of Transportation (5).

Eschenroeder (6) describes an adaptation of a larger scale 2-dimensional photochemical model to microscale at-grade roadway applications. For such applications, however, that model has apparently been supplanted by the more powerful GRC model (2). Ragland and Pierce (7) consider only at-grade roadways but incorporate highly realistic wind and turbulence profiles while also considering 3-dimensional effects. One of the most advanced models is described by Hotchkiss and Harlow (8). This model treats systems of streets and cross streets with complex 3-dimensional obstacles. The flow field is determined by solution of the 3-dimensional conservation of momentum equations including viscous effects (Navier-Stokes equations) as described by Hirt and Cook (12). Validations show good agreement with field data. Danard (9) treats at-grade and depressed roadways by assuming 2-dimensional behavior. A limitation of the application described is the assumption of calm winds within the depression. Kondo (10) deals with only depressed or street canyon roadways and considers specifically a vortex wind field between the buildings.

Perhaps a few words should be said about the assumption of vortex flow in a depression. Such flows have been observed in the field by a number of investigators (13, 14). Further the expected consequence of such motion is to cause higher pollution levels on the upwind side of the depression, and this too has been observed. At one time there was a reluctance by some to accept the notion of such a flow pattern. Today, however, the opposite seems to be true; the acceptance or assumption of such flow patterns is excessive. They do not always exist, even for wind perpendicular to the street. Although fluid dynamics theory has long been aware of such vortices in similar flows, e.g., flow past fins in annuli (15, p. 197), their formation is understood to be dependent on both Reynolds number and aspect ratio, i.e., the depression height to width ratio. Accordingly, it is expected that at least for very deep depressions vortices are not always formed, especially near the bottom of the depression. In addition, mobile laboratory measurements by the New York City Department of Air Resources in deep city street canyons have indicated a preference for channeled flow instead, i.e., flow parallel to the canyon. More definitive evidence of this effect has been observed in a monitoring program recently conducted for New York City by Environmental Systems Laboratory, Inc., and will be reported on in the future.

FUTURE MODELING NEEDS: ADVANCEMENT OF THE ART

In trying to construct a list of areas that are in most urgent need of further work and that will also bear the greatest fruit, I found that all items relate in one way or another to one primary overriding need, namely the improvement of input parameter specifications, i.e., wind and turbulence. The mathematics and computer capabilities are already sufficiently powerful to handle most problems of interest. In complex 3-dimensional cases with highly irregular terrain and man-made obstacles, computer demands may still be impractical for many engineering analyses. However, the development of improved math schemes and computer programs to reduce computer requirements is an area of active research and steady progress.

The great power of numerical models is their ability to account for the complexities of wind and turbulence distributions in the real world; unfortunately, this is also the major source of difficulty, for it requires determination of those distributions. Especially difficult is the determination of the turbulent diffusion coefficients. This has been, and still is, the central problem of turbulence theory. The use of improperly specified wind and turbulence can cause gross errors and is an injustice to the modeling technique. Although it is agreed that wind and turbulence distributions are not easily determined, it is also believed that they are not so mysterious as often alleged and that difficulties are in large part due to a failure to take advantage of existing knowledge. The sciences of fluid dynamics and micrometeorology are not new and have developed a large body of data and methods of analysis for flow around obstacles and over irregular boundaries. This information is readily available in fluid dynamics and micrometeorology texts. Also available in the literature are considerations specifically pertaining to atmospheric flows around obstacles (16, 17, 18). (Scales involved in roadway microscale modeling are at the lower end of, and in some cases smaller than, the scales of classical micrometeorology.) Existing knowledge can be of critical value in numerical modeling, and therefore its exploitation should be a first priority objective. This will be helpful not only in the specification of wind and turbulence but also in the design of more meaningful and effective field measurement programs. This leads to the second need: more field data.

Measurement programs in the past tended to emphasize output, i.e., air quality, while input parameters other than traffic were in general inadequately measured, at least from the point of view of numerical models. Therefore, future measurement programs intended for the development and validation of numerical models should give greater consideration to the wind and turbulence input and should do so in a rational, organized, and optimized way based on the existing knowledge. Such an approach should influence not only the measurement of wind and turbulence but also the placement of pollutant monitors. For purposes of data acquisition as well as improved understanding of the governing phenomena, small-scale physical experiments, as in wind tunnels, should also be more actively pursued. Examples of wind tunnel investigations for atmospheric problems have been published (19, 20, 21, 22). In fact, Hoydysh and Sabetta (22) deal directly with use of wind tunnel results to calibrate numerical models. Although wind tunnel data have been challenged with regard to quantitative validity on the microscale, they can at least reveal qualitative effects and contribute to experiment design for full-scale measurement programs.

Finally, there is an urgent need, and to date a general failure, to be careful. Once models have been developed for particular situations, their limitations should be realized and respected. Subtle changes in terrain or meteorology can have drastic impact on air quality whereas other seemingly major differences in these input factors might have only minor effects on the air. A roadway near an obstacle may cause high pollution near the obstacle while another road only 1 or 2 road-widths farther from the obstacle might have practically no impact at the obstacle. In the first case, the road is contained within a recirculating vortex region formed by the obstacle; in the second case, the road is outside the region. As discussed above, elevated roads with fill are significantly different from those without. Similarly, a depressed road with vertical walls may cause a large eddy to be formed whereas in another depressed roadway, because it is deeper or shallower or has sloped walls, the eddy is not formed. Application of a model developed for vortex flow would give good results in the first case and poor results in the second, not to mention a bad name for numerical models.

Unfortunately many users select a model simply on the basis of general category; e.g., if the user has an elevated roadway, then any model developed for an elevated roadway is assumed applicable. Fault is not only with the user alone but also with the model developer who does not adequately determine and define applicability of the model. To correct this situation as well as to launch a more organized attack on microscale problems, we should investigate and carefully specify the applicability of particular models in terms of quantified ranges of characteristic parameters. These might include geometric parameters such as aspect ratios, roughness heights, and basic shapes and flow parameters such as wind vectors, Reynolds numbers, and Froude numbers. They should cover both the microscale of interest and the larger background scale.

Advancement of the art of numerical modeling is most urgently in need of, and can most effectively be achieved by, improved specification of wind and turbulence fields. To this end it is recommended that the sciences of fluid and atmospheric flows be more thoroughly exploited, that additional data be acquired including field measurements as well as small-scale physical experiments, and that the applicability of models be determined and defined on a more comprehensive and organized basis, with users carefully selecting models accordingly.

NUMERICAL VERSUS GAUSSIAN MODELS

The vast majority of existing microscale models are either Gaussian or numerical (finite difference). Gaussian models are considerably more expedient and less demanding of the computer, but numerical models are more powerful, more realistic, and, therefore, if properly developed and applied, more accurate.

These advantages of numerical models are claimed on the basis that Gaussian equations and numerical models are both solutions of governing partial differential equations (GPDE) for conservation of species, but that the GPDE solved by the Gaussian equation is much less realistic than the GPDE solved numerically. In particular, the Gaussian equation is a solution to the conservation of species GPDE in which the wind and turbulence profiles are both assumed to be uniform in space or more generally where they have the same profiles. Unfortunately, this is unrealistic in the atmosphere except at higher elevations beyond the disturbing influence of obstacles and the boundary layer effects of the ground. On the other hand, numerical techniques, as already discussed, are capable of handling arbitrary wind and turbulence of almost unlimited complexity. Of course, as also pointed out above, use of improper wind and turbulence in numerical models can cause results that are wrong, in fact, possibly much worse than Gaussian results. Thus, it seems fair to say that numerical models at least have the potential to produce more accurate results and handle more complex situations than Gaussian models.

As an aside, all models based on physics, as opposed to those based on statistical, empirical, or other grounds, must conserve mass of the species, that is, in the broader sense including sources, sinks, and chemistry. Thus the label "conservation of mass" applies equally to Gaussian models and to numerical models that solve the GPDE for conservation of species. Unfortunately, this label has been adopted for particular types of models only, such as the numerical, with an implied and frequently assumed exclusion of all other models. This is misleading and unfair to other modelers that are also conserving mass. Therefore, it might be wise to completely avoid the term conservation of mass.

The Gaussian model is generally simpler, more expedient, and less burdensome to the computer. The Gaussian equation is a simple functional relation between receptor and source. Total concentration at a single receptor can therefore be evaluated directly by addition of results from separate Gaussian equations, one for each source. Also the effects of variations in meteorology or sources or both are readily evaluated on either a single or a multiple receptor basis. On the other hand, numerical models require mathematical schemes involving complex algorithms, iterations, matrix inversions, and other procedures that are much more difficult to implement than the simple Gaussian relation. Such procedures can also incur problems with convergence and mathematical instability that can be quite difficult to overcome. Further, the mathematical schemes involve an interdependence of receptor points that precludes computation at a single receptor and requires in each case the computation of numerical results for an entire array of grid point receptors.

Considering the advantages and disadvantages of both Gaussian and numerical models, I believe that both should play, as they have in the past, an important role in microscale air quality modeling. However, in light of some of the weaknesses, it might be worthwhile to spend somewhat more of our efforts on other types of models. Existing techniques and models incorporate some of the advantages of both Gaussian and numerical models without all of the disadvantages. For example, by approximate techniques such as iterative, asymptotic, and weighted residual methods, it is possible to develop functional relations (algebraic-transcendental equations) that are approximate solutions (i.e., close to exact solutions) to complex GPDEs. Such solutions obtained for GPDEs, which are more realistic and general than the GPDE for which the Gaussian is a solution, would provide models having both the convenience of Gaussian models, i.e., the functional form, and some of the greater realism of the numerical models. Further, exact solutions are already available for more realistic GPDEs. For example, Cresswell and Sutton (23, 24) derive exact solution for the GPDE for an at-grade road and arbitrary vertical power law profiles of wind and turbulent diffusivity. The profiles not only are more representative of atmospheric boundary layers but also lead to the Gaussian solution as a special case. To illustrate, the solution is

$$x = cQ\sigma^{-\frac{n+1}{n}} \exp\left(-\frac{\eta^{\nu}}{\nu}\right)$$

where the wind and turbulent diffusivity are assumed to be

$$u = \beta z^{1/n} \qquad K = \partial z^{1/m}$$

respectively, with n and m being arbitrary constants. In the solution, c is a constant, σ is a function of downwind distance, both given as part of the solution, and

$$\eta = \frac{z}{\sigma}$$

$$\nu = \frac{m - n + 2mn}{mn}$$

For $\nu = 2$, the Gaussian solution is obtained, and further this requires $m = n$, that is, the same profile for both wind and turbulent diffusivity. However, based on the law of conservation of momentum in boundary layers, m cannot equal n except in the special case of $n = 2$. Unfortunately, this value of n is not only restrictive but practically nonoccurring, especially over flat terrain. Thus, the Gaussian solution is based on either an unrealistic profile or a violation of the law of conservation of momentum. Considering a value of $n = 7$, which is more typical of the turbulent boundary layers over flat terrain, it follows from conservation of momentum that $m = 7/6$ and therefore that $\nu = 9/7$, i.e., the turbulent diffusivity is nearly linear and the conservation is closer to exponential than Gaussian. The above is an example of models with more rigorous physics than Gaussian models, yet greater simplicity than numerical models. They should not be ignored.

SUMMARY

Numerical techniques provide a powerful tool for the assessment of transportation-related air quality impacts. They are potentially capable of accounting for meteorology and topography of almost unlimited complexity. This paper presents a description of their basic nature, a discussion of existing capabilities including some particular models, suggested ways for improvement of models, and consideration of the relative merits of numerical versus Gaussian models.

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STATISTICAL COMPARISON OF MODEL RESULTS

Paul J. Downey, Transportation Systems Center, U.S. Department of Transportation, Cambridge, Massachusetts

In response to legislation requiring that each federal agency carefully and systematically consider the environmental effects of its actions, the Office of the Secretary of Transportation initiated the Technology for Environmental Analysis (TEA) program at the Transportation Systems Center (TSC) in 1972 to develop unified technological capabilities in air pollution assessment as part of a family of techniques and capabilities necessary to support the Office of the Secretary and the operating administrations in their development of planning procedures related to the environmental impact of transportation systems and facilities.

One important goal of this program is to develop and maintain expertise on the availability, applicability, and performance of techniques for analyzing the environmental impact of transportation-generated air pollution. To aid in the achievement of this goal, TSC has pursued the acquisition of both dispersion models and air quality data. The work reported here is a step toward the fulfillment of this goal.

MODELS TESTED

In the spring of 1974, 13 highway air pollution dispersion models (Table 1) were tested at the Transportation Systems Center by using a portion of the Airedale air quality data base. Six of the models tested were Gaussian, 6 were conservation of mass, and 1 was of another type. Because of the inadequacies in the Airedale data, the original plan to test the accuracy of model predictions had to be abandoned, and instead the approach was adopted of treating the data as a synthetic data sample for use in determining how closely the model predictions agree with one another. The purpose of comparing models in this way is to determine whether the predictions of certain models tend to agree closely, i.e., cluster together.

MODEL CLUSTERING

Consensus models will be defined in this report as those that produce predictions that cluster together. This definition is an interim one, and any conclusions drawn from its application are preliminary, especially when the synthetic sample used is relatively small, as is the case in this study. However, this concept of the consensus models does have the advantage that synthetic data sets can easily be generated for any desired combination of highway geometry, traffic parameters, meteorological conditions, and receptor locations. If it were discovered that similar clusters of model predictions occurred with many different synthetic data sets, then we would have greater confidence in designating the models in these clusters as consensus models. This approach will be pursued until data suitable for model validation become available.

The concept of consensus clusters does have an immediate application to air quality analysis and associated decision making. U.S. Department of Transportation officials must often rely on predictions generated by models when making decisions on the environmental impact of transportation systems. If a model in the consensus cluster has been used for a particular analysis, then the approving federal official can at least be assured that the analysis represents a consensus of several existing models. Similarly, at the state level, highway engineers are often confronted with the task of selecting suitable models for use in computing the air quality impact of proposed highways. Several such models are in the public domain, and others are the property of companies who perform air quality analyses for a fee. Models will differ in the cost of running them (i.e., computations) and in the amount of staff resources that must be allocated to the project. Thus, the cost of using the various models may vary widely. Therefore, information about what models produce similar predictions could result in considerable cost savings in selecting a model for a particular application. Furthermore, if the adequacy of an air quality analysis should be challenged in a court case, the state department of transportation performing the study would be in a stronger position to define it if the model used had been selected from a group that had previously been demonstrated to produce similar predictions.

In the absence of air quality data suitable for testing the accuracy of models, it is impossible to determine whether the predictions of models in a consensus cluster are any more accurate than the predictions of models not in the cluster. Nonetheless, since models within a consensus cluster produce results that agree closely with one another, these models are not likely to harbor theoretical or programming errors in their construction. Furthermore, if the consensus cluster should contain models based on different theoretical formulations, e.g., both Gaussian and conservation-of-mass models (as will be shown to be the case), this fact would lend further credence to the validity of these models within the framework of meteorological theory.

Figure 1 shows a scatter diagram of the predictions of the AeroVironment and Walden Research, Inc., models; these 2 models agree closely. Models that form consensus clusters would be expected to produce predictions that have similar close agreement.

DISTANCE MEASURES

By a pairwise comparison of the predictions of 2 models for the same set of data points, a measure of the "distance" between their predictions can be determined. A model cluster can then be defined as a set of models whose predictions are less than a distance d apart. (The distance d is called the cluster diameter and can be defined as some fraction of the average model prediction.) If there is a single predominant cluster, then that will be called the consensus cluster, and all models in the cluster will be considered to be consensus models. Three types of pairwise model distance measures were used: average absolute difference (AAD), eightieth percentile difference (80%D), and correlation coefficient (CC).

The average absolute difference for 2 models, M1 and M2, can be found by

$$\mathrm{AAD} = (1/N)_{p=1}^{N}\ 'M1(p) - M2(p)'$$

where M1(p) and M2(p) are the predictions of models 1 and 2 for the p th data point and N is the number of points.

Two models can have a low AAD and still have large differences for many data points. Therefore, a second measure, the eightieth percentile difference, is used. This is found by ordering all of the absolute differences, 'M1(p) - M2(p)', and finding the one that is greater than or equal to 80 percent of these differences.

The correlation coefficient measures the tendency of the predictions of 2 models to vary linearly. Thus, a high correlation coefficient indicates a strong linear relation between 2 models, even though there may be considerable absolute difference between their predictions. The correlation coefficient for the pollution predictions (background

Table 1. Models tested.

Company or Agency	Code	Model Type			Testing Mode		Sites for Which Model Was Run	
		Gaussian	Conservation of Mass	Other	Contract	In House	Independence Avenue, Site 11	Military Road, Site 14
AeroVironment	AER		X		X		X	X
California Division of Highways	CAL	X				X	X	X
Center for the Environment and Man	CEM		X		X			X
Environmental Research and Technology	ERT		X		X			X
Environmental Systems Laboratory	ESL	X				X	X	X
General Electric	GE			X		X	X	X
Intera	INT		X		X		X	X
Kaman Sciences Corporation	KAM	X			X		X	X
Lockheed Missiles and Space Company, Inc.	LOC		X		X		X	X
Systems Control, Inc.	SCI	X			X		X	X
System, Science and Software	SSS		X		X		X	X
TSC/EPA	TSC	X				X	X	X
Walden Research, Inc.	WAL	X				X	X	X

Figure 1. Scatter diagram of the predictions of AER and WAL models.

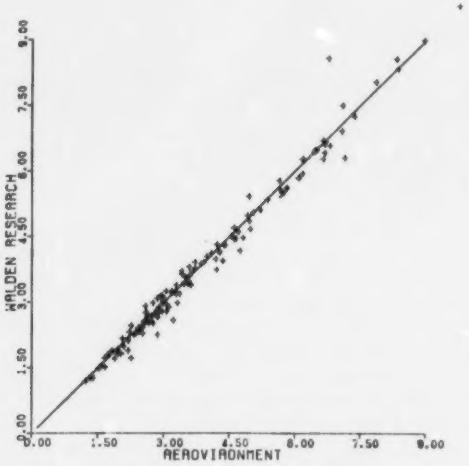


Table 2. Matrix of differences and correlation of model predictions at site 11.

Item	Model	AER	CAL	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL	DAT
Mean absolute difference	AER	0.0	0.24	0.92	3.95	1.66	0.61	0.59	0.98	0.30	0.29	0.20	2.11
	CAL	0.24	0.0	0.87	4.00	1.70	0.59	0.59	1.02	0.34	0.29	0.13	2.19
	ESL	0.92	0.87	0.0	3.62	1.84	0.75	1.35	1.42	0.91	0.80	0.97	2.15
	GE	3.95	4.00	3.62	0.0	4.11	3.84	3.69	3.11	3.96	3.80	3.98	2.74
	INT	1.66	1.70	1.84	4.11	0.0	1.66	1.93	1.89	1.75	1.67	1.71	2.68
	KAM	0.61	0.59	0.75	3.84	1.66	0.0	1.01	1.17	0.72	0.61	0.62	2.1[illegible]
	LOC	0.59	0.59	1.35	3.69	1.93	1.01	0.0	0.86	0.65	0.62	0.51	1.97
	SCI	0.98	1.02	1.42	3.11	1.89	1.17	0.86	0.0	1.04	0.91	0.99	1.49
	SSS	0.30	0.34	0.91	3.96	1.75	0.72	0.65	1.04	0.0	0.35	0.27	2.10
	TSC	0.29	0.29	0.80	3.80	1.67	0.61	0.62	0.91	0.35	0.0	0.28	1.99
	WAL	0.20	0.13	0.97	3.98	1.71	0.62	0.51	0.99	0.27	0.28	0.0	2.16
	DAT	2.11	2.19	2.15	2.74	2.68	2.18	1.97	1.49	2.10	1.99	2.16	0.0
Eightieth percentile difference	AER	0.0	0.30	1.40	5.70	2.60	0.80	0.90	1.30	0.40	0.40	0.30	3.40
	CAL	0.30	0.0	1.60	5.80	2.70	0.70	0.80	1.30	0.40	0.40	0.20	3.40
	ESL	1.40	1.60	0.0	5.30	3.00	1.20	2.00	1.70	1.40	1.30	1.60	3.50
	GE	5.70	5.80	5.30	0.0	6.30	5.70	5.40	4.90	5.80	5.60	5.80	4.20
	INT	2.60	2.70	3.00	6.30	0.0	2.70	2.90	2.70	2.80	2.70	2.70	4.20
	KAM	0.80	0.70	1.20	5.70	2.70	0.0	1.50	1.50	0.90	0.80	0.80	3.40
	LOC	0.90	0.80	2.00	5.40	2.90	1.50	0.0	1.10	0.90	0.90	0.70	3.10
	SCI	1.30	1.30	1.70	4.90	2.70	1.50	1.10	0.0	1.30	1.20	1.20	2.40
	SSS	0.40	0.40	1.40	5.80	2.80	0.90	0.90	1.30	0.0	0.50	0.20	3.40
	TSC	0.40	0.40	1.30	5.60	2.70	0.80	0.90	1.20	0.50	0.0	0.40	3.20
	WAL	0.30	0.20	1.60	5.80	2.70	0.80	0.70	1.20	0.20	0.40	0.0	3.40
	DAT	3.40	3.40	3.50	4.20	4.20	3.40	3.10	2.40	3.40	3.20	3.40	0.0
Correlation coefficient	AER	0.0	0.77	0.75	0.32	0.22	0.65	0.31	0.54	0.76	0.78	0.81	0.23
	CAL	0.77	0.0	0.72	0.27	0.17	0.73	0.42	0.72	0.57	0.67	0.91	0.17
	ESL	0.75	0.72	0.0	0.24	0.25	0.78	0.22	0.39	0.57	0.87	0.69	0.17
	GE	0.32	0.27	0.24	0.0	0.10	0.28	0.38	0.25	0.05	0.31	0.33	0.09
	INT	0.22	0.17	0.25	0.10	0.0	0.28	-0.07	0.08	0.15	0.22	0.15	-0.04
	KAM	0.65	0.73	0.78	0.28	0.28	0.0	0.18	0.50	0.39	0.60	0.68	0.20
	LOC	0.31	0.42	0.22	0.38	-0.07	0.18	0.0	0.50	0.22	0.41	0.57	0.27
	SCI	[illegible]	0.72	0.39	0.25	0.08	0.50	0.50	0.0	0.47	0.43	0.79	0.22
	SSS	[illegible]	0.57	0.57	0.05	0.15	0.39	0.22	0.47	0.0	0.69	0.64	0.22
	TSC	[illegible]	0.67	0.87	0.31	0.22	0.60	0.41	0.43	0.69	0.0	0.71	0.27
	WAL	[illegible]	0.91	0.69	0.33	0.15	0.68	0.57	0.79	0.64	0.71	0.0	0.24
	DAT	[illegible]	0.17	0.17	0.09	-0.04	0.20	0.27	0.22	0.22	0.27	0.24	0.0

removed) of 2 models, M1 and M2, is defined as follows:

$$CC = (1/N)_{p=1}^{N} \{[M1(p) - M1AV][M2(0) - M2AV]\}/[(VAR1)(VAR2)]^{1/2}$$

where

$$M1AV = (1/N)_{p=1}^{N} M1(0),$$
$$M2AV = (1/N)_{p=1}^{N} M2(p),$$
$$VAR1 = (1/N)_{p=1}^{N} [M1(p) - M1AV]^2, \text{ and}$$
$$VAR2 = (1/N)_{p=1}^{N} [M2(p) - M2AV]^2.$$

RESULTS

For each model M the predicted concentration M(p) for each data point p of the reduced Airedale data set was found. Eleven of the 13 models were run for site 11 data, and all 13 models were run for site 14 data.

The outputs of the model runs for all models were used for find difference matrices showing the AAD and the 80%D for all pairs of models for both sites 11 and 14. These and the matrix of the correlation coefficient of model predictions are given in Tables 2 and 3. In these 2 tables, the right column, DAT, pertains to the measured data downwind of the roadway. By all 3 distance measures, the data are far removed from the predictions of all the models, which confirms our contention that these data are not suitable for model validation.

To determine a reasonable cluster diameter distance, the average prediction of all models for all cases was calculated. The difference between the average prediction and the average background is the average predicted pollution contribution of the roadway (which was found to be about 1 ppm). The cluster diameter was then defined in terms of the average prediction. Four clusters were formed with diameters of 0.2, 0.4, 0.6, and 0.8 (i.e., 20, 40, 60, and 80 percent of the average prediction), thereby yielding a series of expanding consensus clusters. In the case of the correlation coefficient, 2 clustering criteria were adopted; 0.75 correlation and 0.65.

The clusters formed by these criteria for each site are given in Table 4. For each site and criterion, the total number of different models that cluster with each model is given in Tables 5 and 6. Finally, Table 7 gives the total over all criteria from the previous tables for each model and distance measure.

The data given in Table 7 show that 4 models, AER, CAL, TSC, and WAL, cluster consistently under all the circumstances considered. Model ERT clustered well at the only site where it was run. The remaining models all failed to cluster as well as the above five. In particular, neither model GE nor model CEM ever clustered with any of the other models. Again it should be emphasized that these results say nothing about the accuracy of the models.

Based on this analysis, 5 models appear to be candidates for the consensus cluster: AER, CAL, ERT, TSC, and WAL. Three of these models are Gaussian (CAL, TSC, WAL) and 2 are conservation of mass (AER, ERT).

A wide variety of computer hardware was used in the running of the models studied here. For example, all in-house runs were made on an IBM 370/155; one contractor used a minicomputer; most contractors used large-scale computers.

The amount of central processor unit (CPU) time used by companies participating in this study varied from a low of 7 seconds to a high of 2,800 seconds. Computer usage data are available for 8 of the models tested in this study (Table 8).

In view of the different hourly rates charged for CPU time and the varying hardware and software used, it would not be fair to compare the CPU costs of the models run under contract. However, all 5 models tested in-house were run on the IBM 370/155; hence there is a comparability basis for these models. Assuming a $700/hour rate (including CPU time, disk I/O, core memory), one could approximate the cost of run-

Table 3. Matrix of differences and correlation model predictions at site 14.

		Model													
Item	Model	AER	CAL	CEM	ERT	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL	DAT
Mean absolute difference	AER	0.0	0.36	3.37	0.39	0.70	2.98	0.41	0.60	0.67	0.71	0.41	0.23	0.37	1.66
	CAL	0.36	0.0	3.68	0.46	0.77	3.25	0.50	0.46	0.52	0.68	0.59	0.24	0.08	1.88
	CEM	3.37	3.68	0.0	3.26	3.11	1.78	3.32	3.62	3.48	3.06	3.23	3.45	3.68	2.41
	ERT	0.39	0.46	3.26	0.0	0.35	2.88	0.22	0.68	0.96	0.87	0.57	0.26	0.47	1.72
	ESL	0.70	0.77	3.11	0.35	0.0	2.87	0.47	0.90	1.29	1.17	0.87	0.59	0.77	1.91
	GE	2.98	3.25	1.78	2.88	2.87	0.0	2.92	3.20	3.04	2.64	2.98	3.02	3.25	2.15
	INT	0.41	0.50	3.32	0.22	0.47	2.92	0.0	0.53	0.91	0.80	0.57	0.30	0.50	1.72
	KAM	0.60	0.46	3.62	0.68	0.90	3.20	0.53	0.0	0.75	0.69	0.78	0.52	0.46	1.85
	LOC	0.67	0.52	3.48	0.96	1.29	3.04	0.91	0.75	0.0	0.64	0.70	0.71	0.52	1.73
	SCI	0.71	0.68	3.06	0.87	1.17	2.64	0.80	0.69	0.64	0.0	0.77	0.69	0.67	1.44
	SSS	0.41	0.59	3.23	0.57	0.87	2.98	0.57	0.78	0.70	0.77	0.0	0.42	0.59	1.58
	TSC	0.23	0.24	3.45	0.26	0.59	3.02	0.30	0.52	0.71	0.69	0.42	0.0	0.25	1.72
	WAL	0.37	0.08	3.68	0.47	0.77	3.25	0.50	0.46	0.52	0.67	0.59	0.25	0.0	1.89
	DAT	1.66	1.88	2.41	1.72	1.91	2.15	1.72	1.85	1.73	1.44	1.58	1.72	1.89	0.0
Eightieth percentile difference	AER	0.0	0.40	4.80	0.60	1.10	4.00	0.60	0.90	0.90	1.00	0.40	0.30	0.50	2.80
	CAL	0.40	0.0	5.20	0.80	1.20	4.40	0.70	0.70	0.70	0.90	0.60	0.40	0.10	3.00
	CEM	4.80	5.20	0.0	4.60	4.50	2.80	4.70	5.00	4.80	4.60	4.60	4.80	5.10	3.90
	ERT	0.60	0.80	4.60	0.0	0.60	4.00	0.40	1.00	1.40	1.00	0.80	0.40	0.80	2.70
	ESL	1.10	1.20	4.50	0.60	0.0	4.00	0.70	1.40	1.90	1.30	1.30	1.00	1.30	2.90
	GE	4.00	4.40	2.80	4.00	4.00	0.0	4.10	4.70	4.20	4.00	4.00	4.10	4.30	3.30
	INT	0.60	0.70	4.70	0.40	0.70	4.10	0.0	0.80	1.30	0.90	0.70	0.40	0.70	2.70
	KAM	0.90	0.70	5.00	1.00	1.40	4.70	0.80	0.0	1.30	0.90	0.90	0.80	0.70	2.80
	LOC	0.90	0.70	4.80	1.40	1.90	4.20	1.30	1.30	0.0	0.90	0.70	1.00	0.70	2.70
	SCI	1.00	0.90	4.60	1.00	1.30	4.00	0.90	0.90	0.90	0.0	0.80	0.90	0.90	2.40
	SSS	0.40	0.60	4.60	0.80	1.30	4.00	0.70	0.90	0.70	0.80	0.0	0.40	0.50	2.60
	TSC	0.30	0.40	4.80	0.40	1.00	4.10	0.40	0.80	1.00	0.90	0.40	0.0	0.40	2.80
	WAL	0.50	0.10	5.10	0.80	1.30	4.30	0.70	0.70	0.70	0.90	0.50	0.40	0.0	3.00
	DAT	2.80	3.00	3.90	2.70	2.90	3.30	2.70	2.80	2.70	2.40	2.60	2.80	3.00	0.0
Correlation coefficient	AER	0.0	0.83	0.54	0.83	0.77	0.40	0.82	0.50	0.17	0.30	0.78	0.85	0.72	0.38
	CAL	0.83	0.0	0.54	0.93	0.90	0.42	0.91	0.58	0.21	0.34	0.73	0.96	0.93	0.35
	CEM	0.54	0.54	0.0	0.41	0.36	0.59	0.45	0.41	0.61	0.48	0.43	0.47	0.49	0.40
	ERT	0.83	0.93	0.41	0.0	0.98	0.32	0.97	0.65	-0.10	0.27	0.74	0.98	0.90	0.30
	ESL	0.77	0.90	0.36	0.98	0.0	0.30	0.95	0.65	-0.18	0.22	0.64	0.96	0.88	0.24
	GE	0.40	0.42	0.59	0.32	0.30	0.0	0.33	0.24	0.40	0.23	0.20	0.36	0.43	0.12
	INT	0.82	0.91	0.45	0.97	0.95	0.33	0.0	0.75	-0.07	0.39	0.72	0.97	0.88	0.33
	KAM	0.50	0.58	0.41	0.65	0.65	0.24	0.75	0.0	-0.13	0.68	0.48	0.62	0.57	0.32
	LOC	0.17	0.21	0.61	-0.10	-0.18	0.40	-0.07	-0.13	0.0	0.25	0.11	0.03	0.12	0.28
	SCI	0.30	0.34	0.48	0.27	0.22	0.23	0.39	0.68	0.25	0.0	0.32	0.29	0.29	0.38
	SSS	0.78	0.73	0.43	0.74	0.64	0.20	0.72	0.48	0.11	0.32	0.0	0.76	0.63	0.41
	TSC	0.85	0.96	0.47	0.98	0.96	0.36	0.97	0.62	0.03	0.29	0.76	0.0	0.93	0.32
	WAL	0.72	0.93	0.49	0.90	0.88	0.43	0.88	0.57	0.12	0.29	0.63	0.93	0.0	0.25
	DAT	0.38	0.35	0.40	0.30	0.24	0.12	0.33	0.32	0.28	0.38	0.41	0.32	0.25	0.0

Table 4. Clustering by differences and correlations at sites 11 and 14.

Item	Site 11 Clusters	Site 14 Clusters
Mean absolute difference		
≤0.2	AER-WAL CAL-WAL	CAL-WAL
≤0.4	AER-CAL-SSS-TSC-WAL	AER-CAL-TSC-WAL AER-ERT-TSC ERT-ESL ERT-INT-TSC
≤0.6	AER-CAL-SSS-TSC-WAL AER-CAL-LOC-WAL CAL-KAM	AER-CAL-ERT-INT-SSS-TSC-WAL AER-CAL-LOC-WAL CAL-LOC-WAL ERT-ESL-INT-TSC
≤0.8	AER-CAL-KAM-SSS-TSC-WAL AER-CAL-LOC-SSS-TSC-WAL ESL-KAM-TSC	AER-CAL-ERT-ESL-TSC-INT-WAL AER-CAL-ERT-INT-KAM-SSS-TSC-WAL AER-CAL-INT-KAM-SCI-SSS-TSC-WAL AER-CAL-KAM-LOC-SCI-SSS-TSC-WAL
Eightieth percentile difference		
≤0.2	CAL-WAL SSS-WAL	CAL-WAL
≤0.4	AER-CAL-TSC-WAL	AER-CAL-TSC AER-SSS-TSC CAL-TSC-WAL ERT-INT-TSC
≤0.6	AER-CAL-SSS-TSC-WAL	AER-CAL-SSS-TSC-WAL AER-ERT-INT-TSC ERT-ESL
≤0.8	AER-CAL-KAM-TSC-WAL AER-CAL-SSS-TSC-WAL CAL-LOC-WAL	AER-CAL-ERT-INT-SSS-TSC-WAL CAL-INT-KAM-TSC-WAL CAL-LOC-SSS-WAL ERT-ESL-INT SCI-SSS
Correlation coefficient		
≥0.75	AER-CAL-WAL AER-ESL-TSC AER-SSS ESL-KAM SCI-WAL	AER-CAL-ERT-ESL-INT-TSC AER-SSS-TSC CAL-ERT-ESL-INT-TSC-WAL INT-KAM
≥0.65	AER-CAL-ESL-TSC-WAL AER-CAL-ESL-KAM-WAL AER-SSS-TSC CAL-SCI-WAL	AER-CAL-ERT-ESL-INT-TSC-WAL AER-CAL-ERT-INT-SSS-TSC ERT-ESL-INT-KAM KAM-SCI

Table 5. Number of models clustering by differences and correlations of model predictions at site 11.

Item	AER	CAL	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL
Mean absolute difference											
<0.2	1	1	0	0	0	0	0	0	0	0	2
<0.4	4	4	0	0	0	0	0	0	4	4	4
<0.6	5	6	0	0	0	1	3	0	4	4	5
<0.8	6	6	2	0	0	6	5	0	6	7	6
Total	16	17	2	0	0	7	8	0	14	15	17
Eightieth percentile difference											
<0.2	0	1	0	0	0	0	0	0	1	0	2
<0.4	4	4	0	0	0	0	0	0	3	3	4
<0.6	4	4	0	0	0	0	0	0	4	4	4
<0.8	5	6	0	0	0	4	2	0	4	5	6
Total	13	15	0	0	0	4	2	0	12	12	16
Correlation coefficient											
>0.75	5	2	3	0	0	1	0	1	1	2	3
>0.65	6	6	5	0	0	4	0	2	2	5	6
Total	11	8	8	0	0	5	0	3	3	7	9

Table 6. Number of models clustering by differences and correlations of model predictions at site 14.

Item	AER	CAL	CEM	ERT	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL
Mean absolute difference													
<0.2	0	1	0	0	0	0	0	0	0	0	0	0	1
<0.4	4	3	0	4	1	0	2	0	0	0	0	5	3
<0.6	7	8	0	7	3	0	8	5	2	0	6	8	8
<0.8	10	10	0	8	6	0	9	9	7	8	[illegible]	10	10
Total	21	22	0	19	10	0	19	14	9	8	15	23	22
Eightieth percentile difference													
<0.2	0	1	0	0	0	0	0	0	0	0	0	0	1
<0.4	3	3	0	2	0	0	2	0	0	0	2	6	2
<0.6	6	4	0	4	1	0	3	0	0	0	4	6	4
<0.8	6	8	0	7	2	0	8	4	3	1	7	7	8
Total	15	16	0	13	3	0	13	4	3	1	13	19	15
Correlation coefficient													
>0.75	6	6	0	6	6	0	7	1	0	0	2	7	5
>0.65	7	7	0	8	7	0	8	4	0	1	5	7	6
Total	13	13	0	14	13	0	15	5	0	1	7	14	11

Table 7. Number of models clustering by all distance measures at both sites.

		Model												
Site	Item	AER	CAL	CEM	ERT	ESL	GE	INT	KAM	LOC	SCI	SSS	TSC	WAL
11	Mean absolute difference	16	17	–	–	2	0	0	7	8	0	14	15	17
	Eightieth percentile difference	13	15	–	–	0	0	0	4	2	0	12	12	16
	Correlation coefficient	11	8	–	–	8	0	0	5	0	3	3	7	9
	All distance measures	40	40	–	–	10	0	0	16	10	3	29	34	42
14	Mean absolute difference	21	22	0	19	10	0	19	14	9	8	15	23	22
	Eightieth percentile difference	15	16	0	13	3	0	13	4	3	1	13	19	15
	Correlation coefficient	13	13	0	14	13	0	15	5	0	1	7	14	11
	All distance measures	49	51	0	46	26	0	47	23	12	10	35	56	48
Both	Mean absolute difference	37	39	0	19	12	0	19	21	17	8	29	38	39
	Eightieth percentile difference	28	31	0	13	3	0	13	8	5	1	25	31	31
	Correlation coefficient	24	21	0	14	21	0	15	10	0	4	10	21	20
	All distance measures	89	91	0	46	36	0	47	39	22	13	64	90	90

Table 8. Computer usage.

Company	CPU Time (sec)	Computer Used
System, Science and Software	68	UNIVAC 1108
Lockheed Missiles and Space Company, Inc.	2,600	UNIVAC 1108
Kaman Sciences Corporation	7	CDC CYBERNET 70
Environmental Systems Laboratory	70	IBM 370/155
General Electric	10	IBM 370/155
TSC/EPA	2,300	IBM 370/155
California Division of Highways	60	IBM 370/155
Walden Research, Inc.	2,000	IBM 370/155

Table 9. Deviations of other model predictions from 5 consensus model predictions.

		Model							
Item	Site	CEM	ESL	GE	INT	KAM	LOC	SCI	SSS
Mean absolute difference, ppm	11		0.89	3.93	1.68	0.61	0.58	0.98	0.32
	14	3.49	0.64	3.08	0.79	0.54	0.68	0.72	0.52
Predictions exceeding those of consensus models, percent	11		39.0	99.8	54.5	47.6	68.3	97.0	54.2
	14	99.2	47.1	100.0	62.1	43.3	66.7	82.1	83.8

ning each of the in-house models with the synthetic data set used here. On this basis, model TSC cost approximately $470 to run and model GE cost only $2.

It may be of some interest to relate the remaining models to the 5 consensus models. To do this, we computed the mean absolute difference of the predictions of each of them and the average of the predictions of the 5 consensus models. In addition, the percentage of predictions exceeding the average of the consensus predictions was also calculated for each of the other models. These results are given in Table 9. If the predictions of a model tend to exceed the average of the predictions of the consensus models, then that model may be said to produce conservative estimates of pollution. By this definition, models INT, LOC, SCI, SSS, CEM, and GE all produce conservative predictions. (However, the predictions of models CEM and GE are extremely conservative since they almost always exceed the consensus predictions.)

CONCLUSIONS

1. Five models were tentatively identified as consensus models: AER, CAL, ERT, TSC, and WAL. Of these 5 models, 3 are Gaussian (CAL, TSC, WAL) and 2 are conservation of mass (AER, ERT).
2. When compared to the 5 consensus models, 6 of the remaining 8 models tended to overpredict pollution concentrations (i.e., tended to make conservative predictions).
3. It is important to understand that the models identified here as consensus models are not necessarily more accurate than the other models. Accuracy can only be determined by evaluating the performance of the models on a suitable sample of highway air quality data. Such data do not exist at this time.
4. The kind of evaluation reported here is useful to both federal and state department of transportation officials who are concerned with the air quality impact of transportation. In particular, state highway engineers who select models from the group of consensus models for use in analyzing air quality have a basis for defending their choice in any court case that might arise.
5. This study is a first step toward identifying consensus models. Since no such information is currently available to federal and state agencies, it was decided that these results should be made available, even though they may be significantly altered by future tests. If, as seems likely, no suitable air quality data become available in the immediate future, additional studies using synthetic data for a large range or variables and site configurations will be used to increase the range of applicability of these conclusions.

AIR QUALITY MODELING AT SIGNALIZED INTERSECTIONS

Robert M. Patterson, Technology Division, GCA Corporation, Bedford, Massachusetts

A good deal of effort has been focused in recent years on the problem of estimating the carbon monoxide ambient air quality impact of roadways. This effort has centered around the characterization of motor vehicle pollutant emissions and the dispersion of pollutants in the atmosphere. Emissions have been characterized as coming from vehicles traveling at an average route speed, and hence an average emission strength has been calculated as a function of average speed and VMT on traffic links. This is the approach presented in EPA Publication AP-42 (1), the FHWA program of model SAPOLLUT (2), and the user's manual for model APRAC-1A (3). The subsequent atmospheric dispersion of pollutants has been estimated by numerical integration along the roadway line source of a Gaussian point source plume, the method used in the EPA HIWAY model (4), or by application of the line source formulation of the Gaussian plume assumption, the technique used in a modified form in the FHWA line source model (5, 6) and in model APRAC-1A.

Increasing attention is now being paid, however, to the localized, microscale problem of hot spots of motor vehicle-related pollutants and, particularly, of carbon monoxide. Hot spots generally occur near locations where traffic congestion, slow speeds, and driving mode changes cause high emission densities and high concentrations. One such location is the signalized intersection. The average route speed assumption is inadequate to characterize either traffic movements or the concomitant emissions at signalized intersections.

This paper presents a validated method for handling the intersection problem. The analytical procedure considers both traffic flow parameters and the effects of driving mode changes on emissions, and it has been used to estimate emissions of carbon monoxide from observed traffic at a signalized intersection. The emission estimates have been applied as inputs to the HIWAY model, and the calculated concentrations show good mean agreement with those observed near the intersection.

METHODOLOGY

The main point of the following approach to describing vehicle movements at signalized intersections is the estimation of queue lengths and average idle times for each leg of the intersection. Other techniques are available, such as those of Webster (7) and Newell (8), and these may be more appropriate in some individual cases. The approach presented here, however, has been used as a component in the successful estimation of carbon monoxide concentrations near intersections, and the other techniques are as yet untried.

Emission factors that depend on driving mode as well as on speed are applied to an idealized model of the behavior of queuing vehicles to develop an emission profile for each intersection approach. All vehicles that stop are assumed to decelerate at a constant rate from a constant cruise speed. They queue up with each vehicle occupying an 8-m (26-ft) interval, and then they accelerate at a constant rate back to cruise speed.

The emission profile is calculated by adding the emissions from each vehicle in each interval according to the speed and mode of the vehicle in the interval.

Estimation of Traffic Parameters

Let the length of the red (plus amber) phase of a traffic signal be R, the vehicle arrival rate be q, the number of vehicles queued at the end of the red phase be N, and the number waiting at the beginning of the red phase be M. Then, based on the assumption of random arrivals and no service during R, the distribution of the quantity N - M is (9)

$$\frac{(qR)^k(e^{-qR})}{k!}, \; k = 0, 1, \ldots \tag{1}$$

where k equals N - M.

This is a Poisson distribution with mean qR. Based on the assumption that M = 0, the mean queue length per cycle is

$$\overline{N} = q(\text{vehicles/sec})\; R(\text{sec/cycle}) \tag{2}$$

This formula neglects the possibility of additional queuing during the green phase before the initial queue clears the intersection. This can be accounted for as follows to provide a conservative estimate of the total queue length during a signal cycle. Given that N vehicles are queued at the beginning of the green phase, the distribution of the total number of vehicles N′ that will queue up during the red and green phases before the queue disappears is given by (9)

$$\frac{N}{N'}\,\frac{e^{-N'\rho}(N'\rho)^{N'-N}}{(N'-N)!}, \; N' = N, N+1, \ldots \tag{3}$$

The mean of this distribution is

$$\overline{N}' = \frac{N}{1-\rho} \tag{4}$$

The parameter ρ is the traffic intensity, which equals the mean arrival rate q divided by the mean service rate s during the green phase. Since $\overline{N} = qR$, the mean total number of vehicles queued during a cycle is given by

$$\overline{N}' = \frac{qR}{1 - q/s} \tag{5}$$

To find the mean queue length on an approach to an intersection, q, R, and s or their equivalents must be known. This is accomplished by using the quantity G/C.

The quantity G/C may be used in 2 essentially equivalent ways. One is as the ratio of the volume of traffic on an intersection approach to the capacity of the approach if there were no competing traffic. The other is as the ratio of the length of the green phase of a signal cycle (seconds) to the cycle length (seconds). The volume of traffic on an approach to an intersection is a known, an estimated, or a projected quantity. To compute the approach capacity assuming no competing traffic requires that a desired level of service plus other parameters that relate to turning movements, percentage of trucks, approach width, and location be known or assumed (10). The lengths of the green signal phase and the total cycle length can be readily measured for an existing signal or calculated for a planned signal installation, providing the signal is fixed time. For a demand-actuated signal, the phase lengths must be calculated based on the relative volume demand of opposing approaches to the intersection. The total cycle length must still be known. The following discussion describes this calculation as it was done for this study, and it shows the relationship of the 2 uses of G/C.

As an example of G/C calculations, suppose that all 4 approaches to an intersection with a demand-actuated signal have an unimpeded capacity of 1,600 vehicles/hour. That is, ignoring the signal and the conflicting traffic, each lane approaching the intersection can accommodate 1,600 vehicles/hour at the desired level of service. Suppose further that the signal at this intersection has 2 green phases, one for east-west movements and one for north-south movements. The assumed volumes and the calculated required G/C's are given below.

Phase	Approach	Volume (vehicles/ hour)	G/C
1	East leg	400	400/1,600 = 0.25
	West leg	350	350/1,600 ≈ 0.22
2	North leg	800	800/1,600 = 0.50
	South leg	600	600/1,600 ≈ 0.38

The G/C for the intersection is the sum of the higher G/C for each green phase, or 0.25 + 0.50 = 0.75. The east and north legs are the critical approaches, and they carry the volumes that the signal must accommodate. Assuming that the amber or yellow phase is 0.10 signal cycle, then Y/C = 0.10, and G + Y/C = 0.85 required for the intersection. Since this is ≤1.00, the intersection will operate at the desired level of service.

Now, there is G/C = 1.00 - 0.85 = 0.15 left over to be divided between the 2 phases. When this has been apportioned, the result will be a G′/C′ for each phase, or what is actually provided for each of the phases. Phase 1 is given its proportion of the 0.15 according to its required G/C:

$$\left(\frac{0.25}{0.75}\right)(0.15) = 0.05$$

Hence, for phase 1, $G'/C' = 0.25 + 0.05 = 0.30$. Similarly for phase 2,

$$G'/C' = 0.50 + \left(\frac{0.50}{0.75}\right)(0.15) = 0.60$$

Hence, if the signal cycle length C is 100 sec long, phase 1 will be (0.30)(100) or 30 sec, and phase 2 will be (0.60)(100) or 60 sec long. Note that G and C are now defined as the length of the green phase and the cycle length respectively. The previous meanings of demand volume and unimpeded capacity that were applied to G and C were used to determine how the demand-actuated signal would apportion the total cycle time to the 2 green phases.

The service rate s (vehicles/second) during green in equation 5 is nearly equivalent to the denominator used to compute the quantity G/C as described above. (Actually it will be slightly less, since there is some delay associated with getting the queue in motion. This leads to a tendency to underestimate $\bar{N}'$.) The volume parameter q (vehicles/second) is the actual volume using the roadway, and it is equivalent to the numerator used to calculate G/C. Hence at level of service E (capacity), 1 - G/C can be used for 1 - q/s.

For a demand-actuated signal, the length of the red (plus amber) phase, R, is given by R (seconds) = (1 - G′/C′) cycle length (seconds). The quantity G′/C′ is the actual green time to cycle length ratio provided at an approach to an intersection, as opposed to G/C, which is the green time to cycle length ratio required to accommodate traffic on an approach as discussed above. Thus, the mean total queue length can be computed by

$$\bar{N}' = \frac{(\text{V vehicles/hour})(1 - G'/C')(\text{cycle length})}{(3{,}600\ \text{s/hour})(1 - G/C)} \qquad (6)$$

Including the amber time with the red time as 1 - G′/C′ is a conservative estimate that assumes nonaggressive driver behavior.

For a fixed-time signal, G/C will be constant for an approach, and this is used in place of G′/C′ used above to compute the length of the red (plus amber) phase. For this case,

$$\bar{N}' = \frac{(\text{V vehicles/hour})(1 - G/C)(\text{cycle length})}{(3{,}600\ \text{s/hour})\left(1 - \dfrac{\text{V vehicles/hour}}{\text{C vehicles/hour of green}}\right)} \qquad (7)$$

Estimation of Emission Parameters

A signalized intersection resolves conflicts between opposing streams of traffic by alternately blocking and then allowing free passage of vehicles on intersecting approaches. This feature, plus the relatively fine detail in emission strength variations that must be known to assess nearby concentrations adequately, implies that the widely used average route speed method of computing emission strengths is not suitable in this case. A detailed knowledge must be provided of the emission variations from a vehicle undergoing mode changes from cruise through deceleration to idle and acceleration back to cruise. The recently developed Modal Analysis Model (11) supplies this emission detail.

The modal analysis model computes total emissions of hydrocarbons, carbon monoxide, and oxides of nitrogen from a user-specified vehicle mix through 1971. Any desired driving sequence falling within the range of model applicability may be used. The model was modified for present purposes to calculate emissions at equal (8-m) length intervals for a given approach cruise speed, rate of deceleration, rate of acceleration, and departure speed for an average vehicle representing a 1974 low-altitude mix. A 1974 mix was obtained by calculating emissions for a 1971 mix based on Table 3.1.2.7 of Report AP-42 (1) and multiplying the results by the ratio of 1974 to 1971 test results. For carbon monoxide this ratio is 39/47. Figure 1 shows the carbon monoxide emission profile calculated by the modified modal analysis model for 1 vehicle decelerating from 56.3 km/h (35 mph) at 1.23 m/s^2 (2.75 mph/sec) and accelerating from 0 back to 56.3 km/h at 1.12 m/s^2 (2.50 mph/sec) with no idle time. These values of speed, deceleration, and acceleration are representative of the values observed at an intersection near a large regional shopping center in Oak Brook, Illinois (12).

The emissions from a single vehicle traveling at an average route speed of 32.2 km/h (20 mph) are also shown. The units on the abscissa are meters upstream (negative values) and downstream (positive values) from the intersection stop line, which,

Figure 1. CO emission profile calculated by modified modal analysis model.

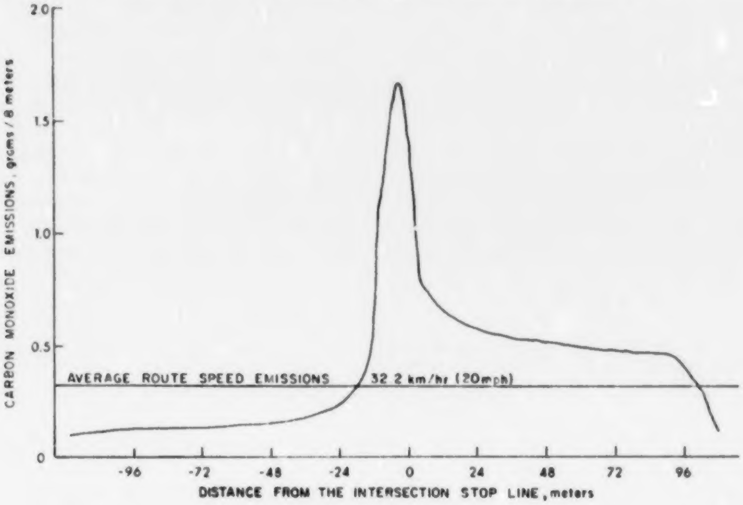
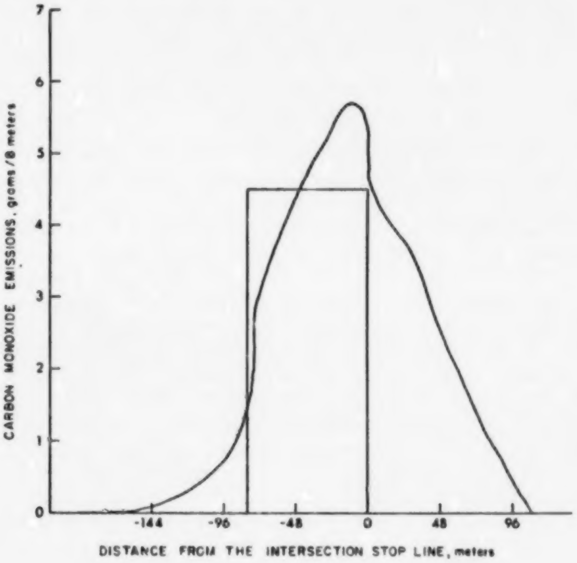


Figure 2. Profile and step function approximation of excess emissions for a queue of 10 vehicles.



for the single vehicle depicted here, is approximately the location of the front bumper when the vehicle is stopped. The vehicle moves from left to right. The ordinate units are g/8 m. Time is not included here, but it will be later in the discussion of applications of the procedures. All that is of interest at this point is the mass of CO emitted in each 8-m length interval by a stopping and starting (but not idling) vehicle.

The emission profile shown in Figure 1 for 1 vehicle is the starting point for developing the emission profile for a queue. It is convenient to consider the emission profile as being the sum of 3 components: excess emissions, idle emissions, and cruise emissions. The excess emissions are those that are attributable to deceleration and acceleration and that are in excess of those occurring at cruise speed.

As stated previously, all vehicles that stop are assumed to decelerate at a constant rate from a constant cruise speed. They queue up with each vehicle occupying an 8-m interval, and then they accelerate at a constant rate back to cruise speed. The emission profile for a queue is developed by adding the emissions from each vehicle in each interval according to the speed and mode of the vehicle in the interval. It consists essentially of adding up $\overline{N}'$ of the curves shown in Figure 1, with each successive curve displaced -8 m from the previous curve, i.e., 8 m upstream. Subtracting the cruise emission component gives the excess emission component for the queue for each length interval along the roadway.

Figure 2 shows the excess emission profile due to stopping and starting only for a queue of 10 vehicles having approach and departure speeds both equal to 56.3 km/h, deceleration of 1.23 m/s^2, and acceleration of 1.12 m/s^2. The scales on the ordinate and the abscissa are different from those in Figure 1. The emission profile shown in Figure 2 does not include idle or cruise emissions, but only the emissions in excess of cruise emissions occurring for stops and starts. The step function also shown in Figure 2 depicts an approximation to the profile of excess emissions. The amplitude equals the average emissions over the queue length of 10 vehicles, or 4.5 g. This average amplitude is 70 percent of the peak value of 5.7 g of carbon monoxide, and the area contained within the step function is 56 percent of the total excess emissions attributable to deceleration and acceleration. The step function approximation is introduced here because it can be conveniently presented and because it is an important aspect of the application to carbon monoxide concentration estimates discussed later.

The excess emissions described here are related to a spatial scale rather than to a temporal scale directly. They arise from 2 effects. This first is an increase in calculated emission rate during both deceleration and acceleration compared to the emission rate at cruise speed. The second is an increase in the time for a vehicle to travel 8 m during deceleration and acceleration compared to the time to travel 8 m at cruise speed. The emission profiles show the product of these 2 effects.

The method of constructing the emission profile for the 10 queuing vehicles and the calculation of the amplitude of the step function approximation are further explained by Table 1, which gives the emissions calculated by the modal analysis model from each of the 10 vehicles in each of the 8-m scale lengths through which the vehicles decelerate and accelerate. The distances from the intersection stop line represent the midpoints of the scale lengths, so that the first queuing vehicle occupies the scale length having its midpoint -4 m from the intersection stop line. Cruise emissions are 0.119 g/8 m.

Data for vehicle 1 show that it travels at cruise speed until it reaches the scale length with midpoint -108 m from the intersection stop line; then it begins to decelerate and the mass emissions/8 m increase. Acceleration emissions from vehicle 1 begin in the scale length with midpoint -4 m; cruising speed is attained again in the scale length having its midpoint at 108 m. Emissions from vehicle 2 are displaced 1 scale length upstream (negative direction) from the intersection compared to vehicle 1 because vehicle 2 must begin decelerating 1 scale length earlier to come to a stop in the scale length immediately behind vehicle 1. Likewise, vehicle 3 begins decelerating 1 scale length earlier than vehicle 2 and so on for the remaining vehicles.

Each row represents a scale length and each column gives the emissions from each vehicle in each row, or scale length. Adding across each row gives the total emissions of all vehicles in each scale length. Excess emissions are obtained by subtracting the cruise component from the total emissions; they thus represent the excess emissions

Table 1. Reference data for describing emission profile calculation.

Distance From Intersection Stop Line (m)	Emissions of Vehicles (g/8 m)										Total Emissions (g/8 m)	Cruise Component (g/8 m)	Excess Emissions (g/8 m)
	10	9	8	7	6	5	4	3	2	1			
-188	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	1.190	1.190	0.000
-180	0.126	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	1.197	1.190	0.007
-172	0.136	0.126	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	1.214	1.190	0.024
-164	0.139	0.136	0.126	0.119	0.119	0.119	0.119	0.119	0.119	0.119	1.234	1.190	0.044
-156	0.142	0.139	0.136	0.126	0.119	0.119	0.119	0.119	0.119	0.119	1.257	1.190	0.067
-148	0.146	0.142	0.139	0.136	0.126	0.119	0.119	0.119	0.119	0.119	1.284	1.190	0.094
-140	0.151	0.146	0.142	0.139	0.136	0.126	0.119	0.119	0.119	0.119	1.316	1.190	0.126
-132	0.157	0.151	0.146	0.142	0.139	0.136	0.126	0.119	0.119	0.119	1.354	1.190	0.164
-124	0.166	0.157	0.151	0.146	0.142	0.139	0.136	0.126	0.119	0.119	1.401	1.190	0.211
-116	0.177	0.166	0.157	0.151	0.146	0.142	0.139	0.136	0.126	0.119	1.459	1.190	0.269
-108	0.193	0.177	0.166	0.157	0.151	0.146	0.142	0.139	0.136	0.126	1.533	1.190	0.343
-100	0.219	0.193	0.177	0.166	0.157	0.151	0.146	0.142	0.139	0.136	1.626	1.190	0.436
-92	0.271	0.219	0.193	0.177	0.166	0.157	0.151	0.146	0.142	0.139	1.761	1.190	0.571
-84	0.600	0.271	0.219	0.193	0.177	0.166	0.157	0.151	0.146	0.142	2.222	1.190	1.032
-76	1.676	0.600	0.271	0.219	0.193	0.177	0.166	0.157	0.151	0.146	3.756	1.190	2.566*
-68	0.788	1.676	0.600	0.271	0.219	0.193	0.177	0.166	0.157	0.151	4.398	1.190	3.208*
-60	0.655	0.788	1.676	0.600	0.271	0.219	0.193	0.177	0.166	0.157	4.902	1.190	3.712*
-52	0.591	0.655	0.788	1.676	0.600	0.271	0.219	0.193	0.177	0.166	5.336	1.190	4.146*
-44	0.553	0.591	0.655	0.788	1.676	0.600	0.271	0.219	0.193	0.177	5.723	1.190	4.533*
-36	2.529	0.553	0.591	0.655	0.788	1.676	0.600	0.271	0.219	0.193	6.075	1.190	4.885*
-28	0.512	0.529	0.553	0.591	0.655	0.788	1.676	0.600	0.271	0.219	6.394	1.190	5.204*
-20	0.501	0.512	0.529	0.553	0.591	0.655	0.788	1.676	0.600	0.271	6.676	1.190	5.486*
-12	0.492	0.501	0.512	0.529	0.553	0.591	0.655	0.788	1.676	0.600	6.897	1.190	5.707*
-4	0.486	0.492	0.501	0.512	0.529	0.553	0.591	0.655	0.788	1.676	6.783	1.190	5.593*
4	0.481	0.486	0.492	0.501	0.512	0.529	0.553	0.591	0.655	0.788	5.588	1.190	4.398*
12	0.478	0.481	0.486	0.492	0.501	0.512	0.529	0.553	0.591	0.655	5.278	1.190	4.088
20	0.476	0.478	0.481	0.486	0.492	0.501	0.512	0.529	0.553	0.591	5.099	1.190	3.909
28	0.365	0.476	0.478	0.481	0.486	0.492	0.501	0.512	0.529	0.553	4.873	1.190	3.683
36	0.119	0.365	0.476	0.478	0.481	0.486	0.492	0.501	0.512	0.529	4.439	1.190	3.249
44	0.119	0.119	0.365	0.476	0.478	0.481	0.486	0.492	0.501	0.512	4.029	1.190	2.839
52	0.119	0.119	0.119	0.365	0.476	0.478	0.481	0.486	0.492	0.501	3.636	1.190	2.446
60	0.119	0.119	0.119	0.119	0.365	0.476	0.478	0.481	0.486	0.492	3.254	1.190	2.064
68	0.119	0.119	0.119	0.119	0.119	0.365	0.476	0.478	0.481	0.486	2.881	1.190	1.691
76	0.119	0.119	0.119	0.119	0.119	0.119	0.365	0.476	0.478	0.481	2.514	1.190	1.324
84	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.365	0.476	0.478	2.514	1.190	0.962
92	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.365	0.476	1.793	1.190	0.603
100	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.365	1.436	1.190	0.246
108	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	0.119	1.190	1.190	0.000

*Mean = 4.504 g/8 m

due to deceleration and acceleration without idle emissions or the emissions that would have been obtained if all vehicles had remained at cruise speed. These are the emissions shown in Figure 2; this column of excess emissions shows the 10 emission values from the 10 queue positions that are used to calculate the average emissions for the step function approximation to the emission profile.

Table 2 gives the average excess emissions occurring over the distance occupied by various lengths and approach and departure cruising speeds. Also given are the standard deviation for each of the average excess emission values to indicate the range of emission values that are used to compute the average. For example, the brace on the right of Table 1 shows the emission values used to calculate the average value of 4.504 g/8 m. These can be compared with data in Table 2, which show, for a cruise speed of 56.3 km/h and a queue of 10 vehicles, an average excess emission value of 4.504 g/8 m with a standard deviation of 1.077 g/8 m. Table 2 also gives the total excess emissions (defined by the entire excess emission profile) contained within the step function approximation. The last column in Table 1, Excess Emissions, totals to 79.930 g. Of this, 45.040 g or 56 percent is accounted for over the 10 queue positions. This percentage is basically a function of the queue length and the distance required to stop and start. The greater the ratio of the queue length to the stop and start distance is, the greater will be the percentage of the total excess emissions contained within the step function.

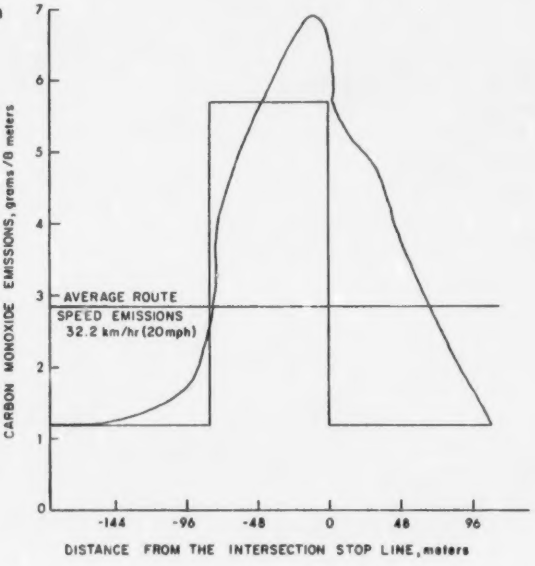
Emissions from cruise and idle modes must be added to those due to stopping and starting to develop the full emission profile. Cruise emissions are included simply by adding the cruise emissions from each vehicle in each 8-m interval. Figure 3 shows the result of adding cruise emissions to the emission profile and to the step function approximation for a queue of 10 vehicles. The profile approximation now contains 68 percent of the total emissions, and the approximated peak of 5.69 g is 83 percent of the

Table 2. Emission values for use in approximating emission profiles.

Speed (km/h)	Queue Length (vehicles)	Average Excess Emission (g/8 m)	Standard Deviation (g/8 m)	Percentage of Total Excess	Total Excess per Vehicle	Cruise Emission (g/8 m)
24.1	5	2.297	0.314	89.3	2.574	0.245
	10	2.436	0.255	94.6		
	15	2.482	0.216	96.4		
	20	2.505	0.190	97.3		
	25	2.519	0.171	97.9		
	30	2.528	0.157	98.2		
32.2	5	2.860	0.533	77.2	3.703	0.183
	10	3.282	0.577	88.6		
	15	3.422	0.492	92.4		
	20	3.492	0.440	94.3		
	25	3.535	0.401	95.5		
	30	3.563	0.370	96.2		
40.2	5	3.066	0.565	61.6	4.978	0.150
	10	3.984	0.866	80.0		
	15	4.315	0.857	86.7		
	20	4.481	0.792	90.0		
	25	4.581	0.734	92.0		
	30	4.647	0.684	93.3		
48.3	5	3.163	0.565	49.4	6.406	0.131
	10	4.389	1.077	68.5		
	15	5.061	1.237	79.0		
	20	5.397	1.215	84.3		
	25	5.599	1.157	87.4		
	30	5.733	1.096	89.5		
56.3	5	3.221	0.565	40.3	7.992	0.119
	10	4.504	1.077	56.4		
	15	5.541	1.521	69.3		
	20	6.154	1.643	77.0		
	25	6.522	1.637	81.6		
	30	6.767	1.590	84.7		
64.4	5	3.253	0.565	33.4	9.745	0.113
	10	4.569	1.077	46.9		
	15	5.679	1.561	58.3		
	20	6.645	1.983	68.2		
	25	7.265	2.114	74.6		
	30	7.678	2.128	78.8		
72.4	5	3.269	0.565	28.0	11.671	0.109
	10	4.601	1.077	39.4		
	15	5.727	1.561	49.1		
	20	6.773	2.051	58.0		
	25	7.719	2.484	66.1		
	30	8.378	2.647	71.8		
80.5	5	3.272	0.565	23.8	13.777	0.108
	10	4.610	1.077	33.5		
	15	5.740	1.561	41.7		
	20	6.790	2.051	49.3		
	25	7.806	2.556	56.7		
	30	8.764	3.029	63.6		

Note: Deceleration = 1.23 m/s² (2.75 mph/sec); and acceleration = 1.12 m/s² (2.50 mph/sec).

Figure 3. Emission profile and step function approximation for excess and cruise emissions for a queue of 10 vehicles.



peak of 6.90 g. When idle emissions are included in the full approximation, these percentages rise to about 95 percent.

Average route speed emissions for 32.2 km/h (20 mph) are also shown on Figure 3. The inclusion of idle emissions, like that of cruise emissions, is a simple calculation and is presented in the following discussion.

APPLICATION OF THE ANALYTICAL PROCEDURES

In this section, an example application of the traffic and emission estimation procedures is given, tying them together to derive inputs for a dispersion model. The results of the application of the procedures to estimating carbon monoxide concentrations at a signalized intersection are then presented.

Approximation of Emission Profiles for Queuing Vehicles

As an example (12), consider an approach to an intersection with a volume of 215 vehicles/hour, $\overline{G}/C$ equal to 0.18, a cycle length of 180 s, G + Y/C of 0.86, and G′/C′ of 0.18/0.76 or 0.24. The mean total queue length per cycle is then

$$\overline{N}' = \frac{(215)(1 - 0.24)(180)}{(3600)(1 - 0.18)} = 10 \text{ vehicles/cycle}$$

The length of the red (plus amber) phase for this example is 138 s. On the average, a stopped vehicle waits one-half of the red phase, or 69 s for this case. The idle emission rate of carbon monoxide calculated by the modal analysis model is 0.234 g/s. This is assumed to occur in each of the queue positions an average of 69 out of every 180 s; that is, (1 - G′/C′)/2, or 0.38 of the time. Hence, the idle emissions average 0.089 g/s for each queue position for this example. This representation tends to underestimate emissions in the lead queue positions, where vehicles wait longer than 1/2 R, and to overestimate emissions for the rear positions.

The HIWAY model calls for emissions in units of grams/meter-second; and now that volume and signal parameters have been specified, these will be calculated for approach and departure speeds of 56.3 km/h, deceleration of 1.23 m/s^2, and acceleration of 1.12 m/s^2. Since $\overline{N}' = 10$ vehicles/cycle, the excess emissions due only to stopping and starting are 4.504 g/8 m/cycle (Table 2), or 0.563 g/m/cycle. But the signal cycle is 180 s, so this becomes 0.563/180 = 0.00313 g/m·s because of stopping and starting. The volume of 215 vehicles/hour equals 10.75 vehicles/cycle for which cruise emissions must be added. The cruise emission rate is 0.119 g/8 m (Table 2), or cruise emissions of

$$\frac{(0.119 \text{ g})(10.75 \text{ vehicles/cycle})}{(8 \text{ m})(180 \text{ s/cycle})} = 0.00089 \text{ g/m·s}$$

The idle emissions were found earlier to be 0.092 g/s for each 8-m queue position, so the idle contribution is 0.01112 g/m·s. The approximation of the emission profile is then

1. 0.00313 g/m·s from stopping and starting,
2. 0.00089 g/m·s from cruise, and
3. 0.01112 g/m·s from idle.

or 0.01514 g/m·s over the 10 queue positions and 0.00089 g/m·s elsewhere. The approximated peak is 95 percent of the peak calculated by using the modal analysis model, and the total approximated emissions are 94 percent of the total. This arises from the large contribution by idle emissions that are computed in the same manner for both cases. The step function approximation neglects excess emissions downstream from the queue. This becomes less important as queue lengths increase, since the high excess emissions during acceleration occur predominantly over the queue positions. This omission is accommodated by assuming that emissions in the center of the intersection equal the mean of the approximated peaks on each approach.

Comparison of Calculated and Observed Concentrations

The modal analysis model and the EPA HIWAY model are designed to estimate emissions and concentrations respectively. To test the compatibility of the 2 models in translating traffic and meteorological parameters into concentrations of carbon monoxide, a composite model was used to predict concentrations for comparison with values observed at a signalized intersection near a regional shopping center.

An exact analysis would include emission strengths calculated for each 8-m section of roadway, application of the HIWAY model to each 8-m section, and addition of the individual section contributions to find the calculated concentration at a receptor. An exact analysis, however, is quite consuming of both staff and computer time; the analysis and results presented here are from a study that determined how well the approximate emission profiles perform with the HIWAY model in estimating carbon monoxide concentrations so that a simple air quality assessment technique could be developed (13, 14). Hence, the approximation technique described earlier was used in obtaining these results.

During a 4-week monitoring program concurrent traffic, carbon monoxide, and meteorological data were collected at a major intersection near a regional shopping center. Figure 4 shows the locations of the carbon monoxide and meteorological monitors, and Figure 5 shows the physical characteristics of the intersection and the locations of the traffic counters. The intersection is controlled by a demand-actuated signal. During this same 4-week period, measurements were also taken of average cruise speeds and deceleration and acceleration rates at various times of the day.

As shown on Figure 4, Ecolyzer carbon monoxide monitors were located at stations 13, 14, 15, and 162. Stations 161 and 163 had NDIR instruments housed in a van, and along with station 162 were operated by the EPA Quality Assurance and Environmental Laboratory. The NDIR instruments were used for comparing and calibrating the Ecolyzer readings to the reference method. The Ecolyzer located at station 162 was changed during the program to ensure that it would not bias the calibration and correction of data taken at the other stations. The calculated and observed concentration comparisons to be presented were based on corrected Ecolyzer readings.

Twelve hours were chosen for analysis based on relatively low wind speed, a wind angle suitable for defining concentrations upwind and downwind of the intersection of Route 83 and Twenty-second Street, and completeness of the input data set for the hour under study. In 4 of these cases the wind was from the northeast quadrant, and concentrations were calculated for the monitor in the southwest quadrant (station 162). In the other 8 cases the wind direction was reversed, and concentrations were calculated for each of the 3 monitors in the northeast quadrant (stations 13, 14, and 15). Missing data occurred for 1 case at station 13 so that there are a total of 27 comparisons of observed and calculated values. Concentrations recorded by the Ecolyzer were used for the southwest location unless it was not operating for the particular hour under study. In these cases the average of the NDIR values (stations 161 and 163) was used. Complete data listings are given in another report (12).

Figure 6 shows a plot of the data pairs. Concentric circles indicate more than one point. Twenty-two calculated values are within a factor of 2 of those observed, and 5 vary by more than a factor of 2. Six of the calculated values agree exactly with the observed values. The average of all calculated concentrations is 3.5 ppm versus 3.8 ppm for the observed average. The correlation coefficient is $r = 0.34$, which indicates less

Figure 4. Continuous monitoring sites at Route 83 and Twenty-second Street.

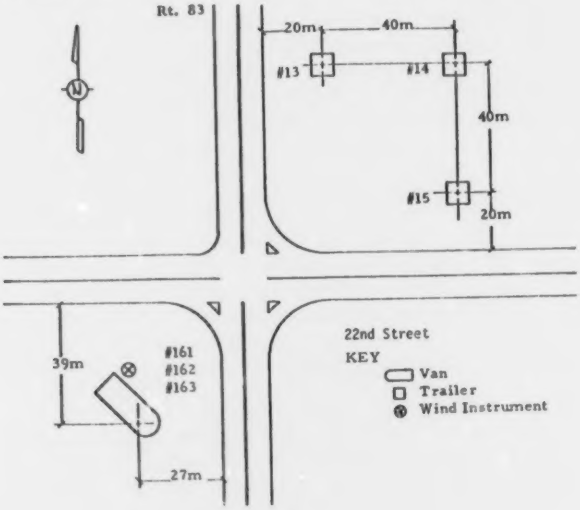

N
Rt. 83
20m
40m
#13
#14
40m
#15
20m
39m
#161
#162
#163
27m
22nd Street
KEY
Van
Trailer
Wind Instrument

Figure 5. Location of traffic counters.

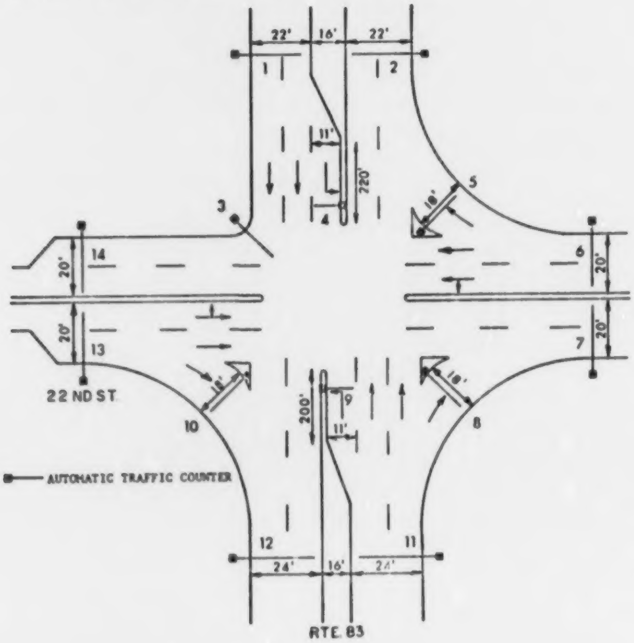
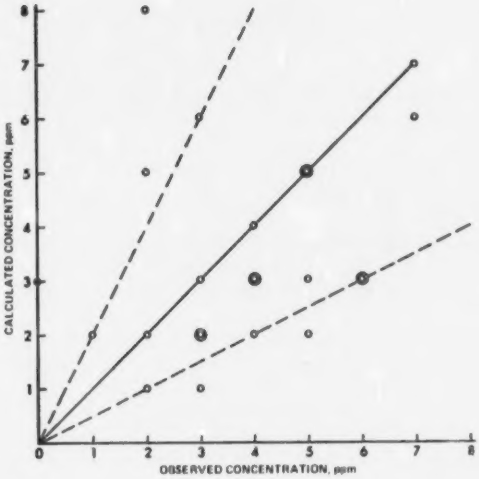

22'
16'
22'
1
2
11'
220'
3
4
5
18'
14
20'
6
20'
13
20'
7
20'
22 ND ST
10
200'
9
11'
18'
18'
8
AUTOMATIC TRAFFIC COUNTER
12
11
24'
16'
24'
RTE 83

Figure 6. Calculated versus observed concentrations of CO.



than a 10 percent probability that the linear relation between calculated and observed values has occurred by chance.

When the values are normalized for wind speed, the mean calculated χU is 11.7 ppm-m/s compared to 13.7 ppp-m/s observed. The correlation coefficient is 0.44, significant at the 2 percent level. Predicted concentrations tend to be overestimated at low wind speeds and underestimated at higher wind speeds. The crossover occurs at wind speeds of approximately 3.5 m/s.

SUMMARY AND CONCLUSIONS

This paper describes an approach for relating the impact of traffic on ambient carbon monoxide concentrations near signalized intersections by (a) computing the emission profiles due to acceleration and deceleration of queuing vehicles for a range of queue lengths and approach and departure speeds, (b) approximating the profiles by simple step functions based on emissions on the portion of roadway occupied by the queues, (c) adding in emission components for cruise and idle modes of vehicle operation, and (d) using the derived emission profiles in a line source dispersion model to estimate ambient CO concentrations at selected receptor sites. The following steps for estimating emission profiles have been suggested and applied successfully.

1. Identify the parameters necessary for calculating the expected mean total queue length. These parameters are V = hourly demand volume, cycle length, G/C = required G/C ratio, G′/C′ = actual G/C ratio provided G/C = actual G/C ratio provided if the signal is fixed time, and capacity per hour of green.
2. Compute the expected mean total queue length using equation 6 for a demand-actuated signal or equation 7 for a fixed-time signal.
3. Round off the calculated queue length to a multiple of 5. If average emission factors are known for the exact queue length, these should be used and it would not be necessary to round off the queue length to a multiple of 5.
4. Identify the approach and departure speeds. If they are unequal, assume that both equal the departure speed. If the average emission factors are known for the given approach and departure speed combination, these should be used and it would not be necessary to make the assumption that both equal the departure speed.
5. Using the data presented in Table 2, find the mean emissions per 8 m due to stopping and starting for the queue length-speed combination.
6. Calculate the emission strength (grams/meter-second) over the distance occupied by the queue by adding the following:

$$\frac{(\text{mean stopping and starting emissions, g/8 m})}{(8\text{ m})(\text{cycle length, second})}$$

$$+\ \frac{(\text{cruise emissions, g/8 m})(V\text{ vehicles/hour})}{(8\text{ m})(3600\text{ s/hour})}$$

$$+ \frac{\text{(idle emission rate, gram/second)(1/2 length of red phase, second)}}{\text{(8 m)(cycle length, second)}}$$

$$= \text{emission strength over the queue length (grams/meter-second)}$$

7. Assume that only the cruise speed emission strength exists upstream and downstream of the queue (excluding the center of the intersection).
8. After the emission strengths are found over the queue lengths for all approaches, average them, and assume this emission strength for lanes in the center of the intersection.

When the above approach was tested by using observed traffic data, it yielded a good estimate of the mean impact on nearby short-term carbon monoxide concentrations. Individual calculated and observed impacts on short-term CO concentrations were generally within a factor of 2 of one another.

This paper focuses heavily on presenting a detailed discussion of an analytical method for modeling the carbon monoxide air quality impact of signalized intersections. The intent is to describe the method fully, so that it may be easily applied by others. A number of comments can be made in conclusion on this topic in general.

1. The basic method is applicable to any vehicle-related pollutant, such as sulfates or lead, for which mode-dependent emission factors are available. In addition to carbon monoxide, the modal analysis model calculates emissions of total hydrocarbons and nitrogen oxides, and these pollutants could be readily modeled. The modal analysis model also calculates fuel consumption.
2. As alluded to earlier, the techniques presented here are not unique, except that they are the first to be applied and validated. They have been applied in the development of the EPA indirect source guidelines document (14).
3. Some of the assumptions used were made for the purpose of simplifying the method, and these can easily be accommodated if a more rigorous application seems warranted. An example is the assumption of constant deceleration and acceleration, which can readily be modified, and new emission estimates can be made based on varying deceleration and acceleration values.
4. The basic methods of simulating traffic, emissions, and dispersion can be applied to nonisolated intersections. Modeling studies that simulated traffic flow, mode-dependent emissions, and dispersion have been made to optimize signal progressions using air quality as the measure of effectiveness (15, 16). Along these same lines, these techniques could be used to include air quality as a measure of effectiveness in designing computer-controlled signal networks.
5. The methods presented in this paper supply the foundation for investigating the impact of traffic engineering practice on air quality. Perhaps contrary to intuition, there are situations in which the goals of the traffic engineer in promoting flow do not lead to good air quality and even cause hot spots (17). Much work remains to be done in the area of intersection modeling to identify these situations and to provide for alternative traffic management techniques that promote both traffic flow and air quality.

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MESOSCALE MODELING: A TRANSPORTATION AGENCY'S EXPERIENCE

George W. Ellis, Urban Planning Bureau, Alabama Highway Department

In recent years the resources applied to air quality model development have increased rapidly. Users are faced with a multiplicity of models more complex and difficult to use. Often a transportation agency lacks the technical skills required to use the models properly, and so model application is growing more slowly than model development. Evidently, the users need help, primarily in the area of input data. The user is told too little about how the data can be obtained, because the model maker is either not qualified to advise on such matters or considers his or her mandate to be only developing the model and fitting it into the planning process. There is a great need for unification.

Admittedly, achievement of a synthesis in which the models become unified in the transportation planning process is difficult, but the potential for model synthesis is no less exciting than that for model development. The state of the art of computer science today with respect to hardware vis-à-vis software is reversed from the situation of only 10 or 15 years ago. Machines then placed severe restrictions on the model maker and the model user. The machines of today, however, defy us to use them fully, and this gap between hardware and software will probably continue into the foreseeable future. I will examine some of the mesoscale models and describe the experiences of using them in Alabama.

DIFFUSION MODELING: APRAC-1A

The APRAC-1A urban diffusion model computer program, developed by the Stanford Research Institute, estimates concentrations of carbon monoxide resulting from the emissions from a traffic network at specified receptor locations under specified weather conditions. Required input for the model includes emission factors, traffic distribution, and meteorological data. Estimates can be made for any time of the day and any day of the year. An option of the model allows estimates of the street canyon effect. Use of the model for developing isopleth contour maps is made possible by means of the grid point mode in which estimates for a given hour of the day are made at a large number of receptor locations (1).

Receptor Spacing

For developing isopleth contour maps, receptor spacing must be sufficiently close for high resolution of the resulting concentrations. To determine just how close this spacing should be, a number of test runs were made with the APRAC in which St. Louis network data were used as input under synthetic worst case conditions (164-ft or 50-m mixing depth, 1-knot or 0.5-m/s wind speed). Results indicated that spacing should be no greater than 328 ft (100 m), and 164 ft (50 m) is preferred. The automatic receptor generator was used, and for this study spacing down to 10 m was used; a maximum of

25 ppm resulted with 1972 emission factors. In general, the greater the spacing is, the lower is the probability of generating concentrations close to the maximum. Obviously, for high resolution isopleths, very large numbers of receptors must be generated and automatic generation is essential. Random spacing was investigated and, based on limited results, appears to have no advantage over fixed spacing. Conceivably, however, a Monte Carlo approach could be devised and incorporated in the model by using a search algorithm, thus reducing the output substantially.

The automatic receptor generator has been incorporated as a modification of the APRAC. In its original form, the program requires 1 card per receptor. When the objective is to develop isopleth contours, the number of receptor cards may be large, requiring a prohibitive amount of work even for the smaller urbanized areas. The modification is available as an option and should be used only if the receptors are to be spaced evenly and the area containing the receptors is a square or a rectangle. The option should not be used for the street model mode. The A card specifies whether the option is to be used. The B card provides information required for the automatic generation of receptors, i.e., the minimum and maximum x and y values and the desired x and y spacing of receptor locations. The modification also includes a change in subroutine PPDATA (the output subroutine), such that the receptor coordinates are printed out along with the other information. This change applies to all options of the program. In addition, the model was modified so that receptor locations are specified in metric units.

Traffic Input Data

Obviously, no model can be more accurate than the traffic used for input. Machine counts or manual counts are used for those systems for which counts are available. For forecast years, traffic density is estimated by using those techniques that are a part of the transportation planning process. To reduce the manual effort required to develop the network data, the state developed a utility program that reads from the magnetic files containing the raw network data, performs the required conversions, and punches network cards (the N cards used as input to the APRAC-1A).

Speed-delay studies have been made in the city of Montgomery. Speeds on every link of the network were measured, both during peak-hour travel and off-peak. If resources allow, these studies will be extended to the other cities of Alabama; and if the results appear to be valid, then these speeds will be used in air quality studies rather than the synthetic speeds resulting from the assignment process.

Weather

Weather is, of course, an indispensable consideration in developing and using diffusion models, and it is well that models have the capability of considering any type of weather. However, those who develop and use air quality reports and those who must devise control strategies from them are primarily interested in worst case conditions—weather, traffic, or otherwise—since such a set of conditions will determine whether the air quality standards will be met or violated. The model maker should consider the ease or difficulty required in obtaining weather data. The state has developed a modification of the APRAC that improves ease of operation without degrading the power and sophistication of the model. Following is a description of the modification.

A required input to the APRAC in its original form is upper air (radiosonde) data [the temperature and pressure up through the 500-millibar (100-kPa) level]. Such data are difficult to obtain for most users, and forecasting these data for the future would be impossible without professional meteorological advice (difficult to obtain, to say the least). In 1973 the Alabama Air Pollution Control Commission recommended that the program be modified so that the need for the upper air data could be eliminated and the minimum and maximum mixing heights be input instead. This proved to be a feasible and rather easy modification to make. In the original program, the upper air data, from the Q cards, are used (in SUBROUTINE RAOBHM) to compute the minimum and maximum mixing heights HMIN and HMAX. Then HMIN and HMAX are used to compute the hourly mixing heights. The modification consists of bypassing that part of SUBROUTINE RAOBHM that reads in the upper air data and computes the HMIN and HMAX. Then HMIN and HMAX are added to the read statement for the P cards. To use the modification requires that Q cards be eliminated and HMIN and HMAX be added to the P cards. The output of the modified program is unchanged from that of the unmodified version except that the number of RAOB levels is not included. Mixing heights for specified areas can be obtained from the literature (2, 3).

Since the intent has been to use worst case conditions and since wind direction is an important factor in determining these conditions, a method was developed to rotate the wind vector at 30-deg intervals around the compass so that a total of 12 runs is required for the study. This method was used for a 3 × 3-mile (4.8 × 4.8-km) area of the central part of Mobile, where receptors were placed 0.1 mile (0.16 km) apart and the highest concentrations at each receptor of all 12 runs were recorded and then contoured (Figures 1 and 2). The importance of wind direction is indicated by the fact that the highest level estimated is 20 ppm with the prevailing southerly wind and 34 ppm with

Figure 1. Contours of highest CO concentrations of 12 receptors with south wind.

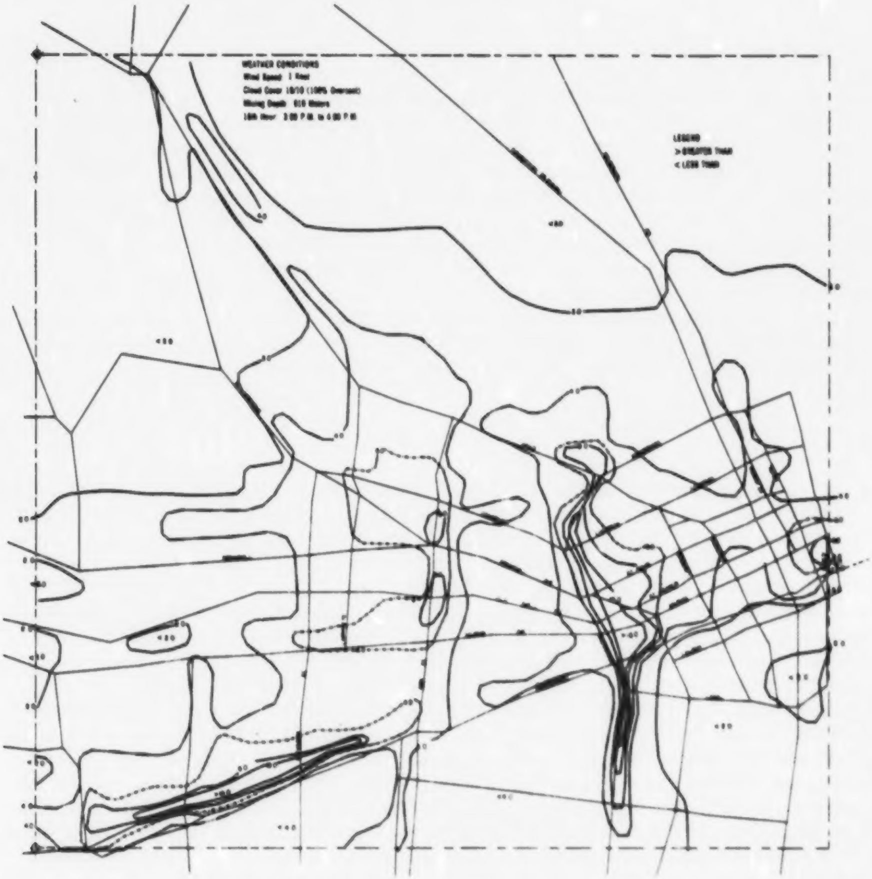


Figure 2. Contours of highest CO concentrations of 12 receptors with rotated wind.

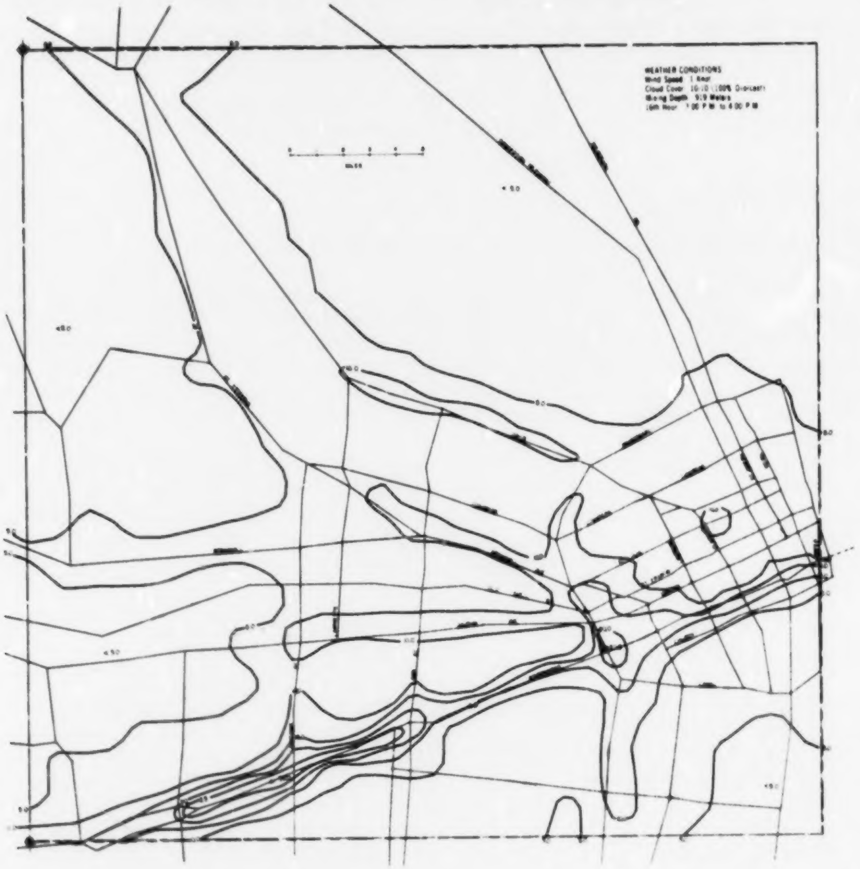
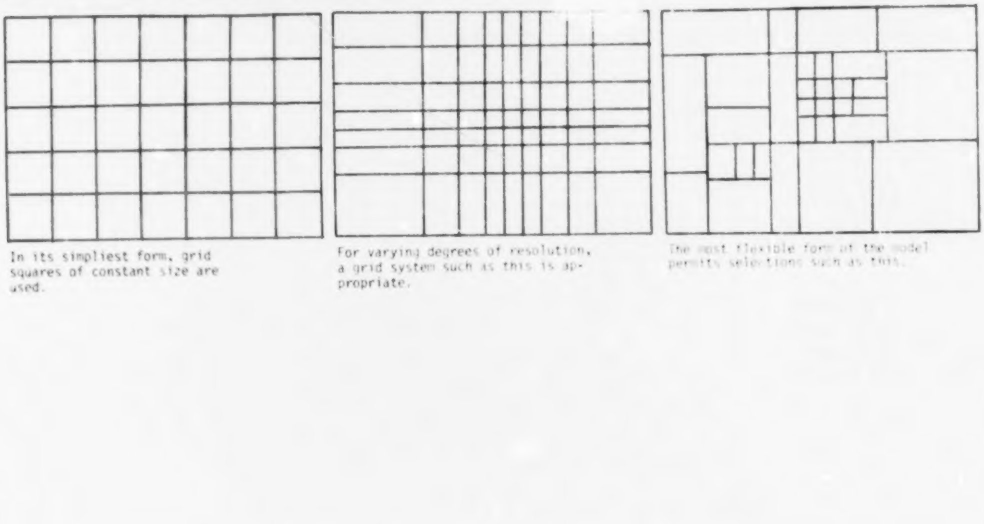


Figure 3. Emission inventory grid systems program (GRIDSUM).



In its simpliest form, grid squares of constant size are used.

For varying degrees of resolution, a grid system such as this is appropriate.

The most flexible form of the model permits selections such as this.

the rotated procedure. The use of the rotated wind, together with worst case traffic and stable air conditions, will probably yield levels higher than actual monitored levels and is therefore of value in determining the potential that high concentrations will occur in an area rather than the probability that they might occur. An unexpected result of the studies was that highest concentrations were estimated for Mobile, not Birmingham. This phenomenon occurs because the Mobile street system is more congested than the Birmingham street system, resulting in significantly lower speeds.

Application of the Model

The APRAC-1A has been run for 6 urbanized areas in Alabama and will be used as additional areas are added. It was used in air quality studies that were issued first in 1974 as a part of the certification of the transportation planning process. In general, the state plans to update its air quality studies only when there are significant changes in any of the factors affecting the studies, such as emission factors, traffic projections, or improvements in air quality modeling. Each air quality report has been reviewed by the Alabama Air Pollution Control Commission to determine the consistency of the report with the state's Air Quality Implementation Plan, and the letter of review has been included as a part of the report.

Figures 1 and 2 show examples of isopleth contour maps of Mobile that were developed by using outputs of the APRAC-1A. The APRAC-1A was run in the street canyon mode for 1 street in Mobile and 9 streets in Birmingham. Since the ratio of building height to street width is less than one, the estimates probably tend to be high. Highest concentrations were found to be virtually independent of wind direction and were about 10 ppm in Mobile and 30 ppm in Birmingham.

Data Processing Considerations

For the benefit of anyone who anticipates using the APRAC model, some information relating to the actual processing follows. In its original form, the program is dimensioned for 625 receptors (grid point mode) and 1,200 network links. It is fairly easy to redimension the program to increase its capability by changing the number of receptors and links at all places where they occur in the appropriate COMMON statements of the main program and the subroutines. XPT, YPT, and CCAL must be dimensioned for the number of receptors and ISK, X1, X2, Y1, Y2, and E must be dimensioned for the number of links. Also, in SUBROUTINE SFCOB2, 1200 must be changed in the initializing DO statement just before statement 40 if the number of receptors is to be changed. Execution of the program on the Alabama Highway Department IBM 370, as originally dimensioned, required 125 K bytes of storage, not including system overhead requirement (8 K to 12 K for the IBM 370 machine). Some typical program execution times on the IBM 370 are as follows (times do not include compilation):

Mode	Period (days)	Receptors	Links	CPU Time (min, sec)
Synoptic	30	6	1,371	35, 14
Synoptic	1	9	445	1, 5
Grid point	1	328	834	2, 10
Grid point	1	622	834	3, 18
Grid point	1	328	1,316	3, 34
Grid point	1	622	1,316	5, 12
Grid point	1	1,288	856	7, 13
Grid point	1	884	454	3, 13
Grid point	1	1,219	3,330	24, 50

Obviously, to reduce computer time, runs involving many days of input data should be avoided. For the grid point runs summarized above, times varied from 367 to 496 μsec/receptor/link.

For those using machines that are operating in a multiprogramming environment, simultaneous runs can be made with different wind directions. To do this, one should have all the weather cards ready in advance (one set of R cards for each wind direction) and then change the R cards on each successive pass into the card reader. Each run corresponding to one wind direction drops into a separate partition and runs independently of the others. In this way, as many as 6 wind directions have been run simultaneously, and jobs run for 12 wind directions as described above even with large numbers of receptor points have been completed in less than 90 min clock time. By comparison, more than 6 hours would be required for sequential runs using the same input data.

Part of the data input for the APRAC is the network card deck, which can be quite large for large networks. A fairly simple modification to the APRAC allows the model to read the network data from a disk file, thus eliminating the physical problem of manipulating the N cards. The state has incorporated such a modification as an option. A few changes in subroutine INDAT are all that is required.

Critique

The most serious shortcoming in using the APRAC-1A is that the emission factors used are not the same as those required for other models, but rather are curve-fitting constants alpha and beta. If the model is to be widely used, it should be modified so that emission factors such as those in Publication AP-42 can be used.

The extraurban contribution should be removed from the model since determining the input data is difficult and subject to error. The technique used in the model for calculating this contribution does not contain a provision for changes in emission factors. Therefore, it would be better to use local measurements or estimates for this component.

The APRAC-1A is inherently difficult and costly to use. However, the potential user should realize that after experience with the model, as with any model, he or she will find it is progressively less difficult. Also, further efforts to automate the use of the model should bear fruit. It need not be used often for any given area; every 3 to 5 years would probably be sufficient after thorough initial air quality studies have been made. The model is the most sophisticated of its type available. It would be advisable, therefore, to develop it further and improve its documentation rather than turn to less comprehensive alternatives.

EMISSION INVENTORY MODEL

For spatial resolution of emissions, emissions must be estimated for subdivided portions of an urban area. Alabama has developed a mobile emission inventory model that integrates traffic emissions and other traffic information in a highly flexible technique whose grid systems are shown in Figure 3. The model has been developed as a computer program called GRIDSUM and uses the same traffic input as the APRAC-1A. It estimates daily emissions of carbon monoxide, exhaust hydrocarbons, crankcase and evaporative hydrocarbons, and nitrogen oxides. It also provides a summary of area-wide totals for each pollutant type, vehicle miles traveled, network miles, and capacity miles and has 2 additional options that provide for processing of traffic data for isolating areas of roadway capacity deficiencies.

Figure 4 shows how the output of the model was used to estimate 24-hour emissions for Huntsville, Alabama, using 1-mile^2 (1.6-km^3) grid squares. Square kilometer grids will be used in future reports unless specific occasions require otherwise. Although this model was developed to integrate mobile emissions, a fairly simple modification would add point and area sources to it in order to get an output that would represent

Figure 4. Calculated emission patterns of CO and HC for Huntsville with 1980 street system including I-565.

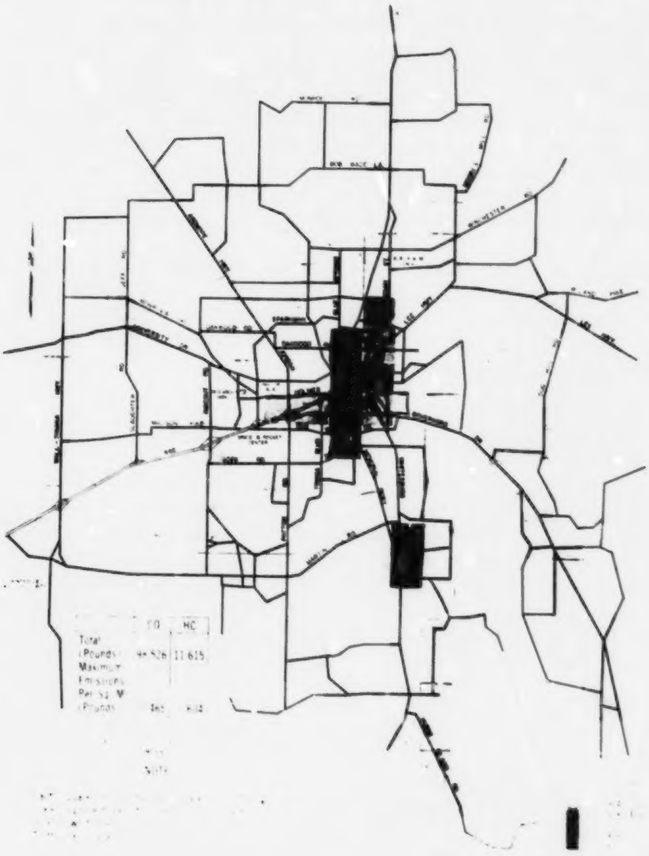
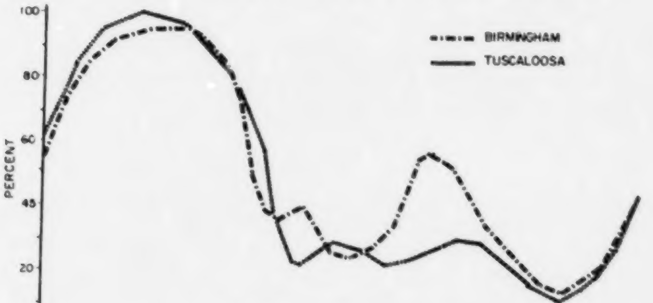

CO
HC
Total
(Pounds)
11,615
Maximum
Emissions
Per Sq. M
(Pounds)

Figure 5. Cold-start profile (percentage of internal trips for each hour).



total (mobile and stationary) emissions. The 3 options available in the program are as follows:

1. Option 1 outputs the emissions of carbon monoxide, exhaust and nonexhaust hydrocarbons, nitrogen oxides, network miles, and vehicle miles for each grid area. In addition, an areawide total of each quantity is output at the end of the report.
2. Option 2 outputs vehicle miles, network miles, capacity miles, and a volume to capacity ratio (V/C ratio) for each grid area. The summary page provides network totals and a percentage breakdown of the grid squares by V/C ratio.
3. Option 3 is similar to option 2 in that both aid in studying street system capacity deficiency. However, in option 3, each link is categorized according to generalized north-south or east-west direction breakdown of traffic flow. The output of each grid area is a separate listing of north-south and east-west vehicle miles and capacity miles and a V/C ratio for each directional category.

The program was developed in FORTRAN IV on the IBM 370/145 with the virtual storage operating system and requires approximately 128 K bytes of storage, not including system overhead. Execution time depends on the number of network links and the number of grid areas selected for summing. For a network of 3,100 links and 900 grid areas (Birmingham), an execution (CPU) time of 1 min and 40 sec was required.

A potentially valuable use for the output of GRIDSUM would be as an input for a dispersion model such as the climatological dispersion model (CDM), which is designed to accept point and area sources. Although GRIDSUM was intended to apply to CO, HC, and NO_x, it can be used for any mobile pollutant for which emission factors are available.

TRIP-MAKING ANALYSIS

According to the EPA equations (4) for carbon monoxide, the 100 percent cold-start correction factor for 1971 and 1972 automobiles at 19.6 mph (31.4 km/h) average route speed is 2.52 and 2.06 for 50 and 75 F (10 and 24 C) respectively. It follows, therefore, that to ignore cold starts is to introduce large uncertainties into our model. (The cold operating mode is defined as the first 505 sec of operation of an automobile that has been in a motor-off condition for 4 hours or more.) To make an accurate assessment of the cold-hot condition, it is essential to study the trip-making process from trip generation and trip distribution to traffic assignment. EPA suggests that 20 percent cold operation be used as an average. However, it is necessary to know what the hourly variation is in urban centers. Accordingly, a study was made of the home interview data taken during the origin-destination surveys in 2 Alabama urban centers: Tuscaloosa and Birmingham. Tuscaloosa is a small city (about 91,000 persons) with substantial light industry and little heavy industry; it is the home of the University of Alabama. Birmingham is a medium-large city (about 615,000 persons), is heavily industrialized, and has a large blue-collar population. The trip data were studied to determine the history of individual vehicles through the day. Results for the 2 cities are shown in Figure 5. The first trip of each day was assumed to be a cold start. Cold starts for all subsequent trips were recorded only when 4 hours or more elapsed from the end of one trip to the beginning of the next. The analysis showed that before 9:00 a.m. about 71 percent of the cold starts occurred in Tuscaloosa and about 40 percent in Birmingham. Note that the profiles for the 2 cities are generally rather similar, particularly with respect to activity during the early and latter portions of each day. However, between 9:00 a.m. and 8:00 p.m., Birmingham is somewhat different; the peaks are higher, and they occur earlier. Cold starts were about 46 percent of the total in Birmingham and 35 percent of the total in Tuscaloosa.

These profiles were derived from a limited amount of data: for Tuscaloosa, about 1,000 trips representing 212 vehicles and 176 households; for Birmingham, about 1,100 trips representing 291 vehicles and 233 households. The state is developing a computer program that will read all the origin-destination survey data for all urban areas in Alabama.

Given sufficient data, one might find that each city would exhibit a distinct signature with respect to its cold-start profile, and it might be possible to generalize these profiles as a function of city size and type. It would be interesting to compare profiles for a large white-collar metropolitan area such as the District of Columbia with a highly industrialized area of comparable size.

Households with more than 1 automobile were studied separately to determine to what extent, if any, socioeconomics affect the cold-start profile. No great difference was apparent. In Birmingham, the multiple-car households exhibited a slightly higher (about 1.5 percent) overall percentage compared with single-car households, and the morning and afternoon peaks were slightly lower. However, the sample size precludes drawing any conclusions. When the computer program is completed, the state plans to study the socioeconomics of trip making in greater detail.

The profiles discussed above are derived only from the condition of a given vehicle at the beginning of each trip and do not consider the vehicle condition during the trip. A complete analysis must consider the length of the trip, for the length will determine how much of the trip will operate in the hot mode. To do this, we must study trip distribution. For example, the effect of the higher cold-start percentage in Birmingham will be offset by the fact that the average trip length is much greater in Birmingham. Therefore, a higher percentage of Birmingham trips that started cold will reach the hot condition. Average trip duration is about 22 min in Birmingham and only about 12 min in Tuscaloosa. Work trips average 31.27 min in Birmingham and 13.13 min in Tuscaloosa. Nonwork trips average 20.92 min in Birmingham and 10.88 min in Tuscaloosa. From the above, we can calculate that about 27 percent of the travel time of the Birmingham work trips that start cold will be in the cold mode and 73 percent in the hot mode (505 sec = 8.42 min ÷ 31.27 = 26.9 percent). Using the same technique, one can calculate that the cold-mode percentages for Birmingham nonwork trips, Tuscaloosa work trips, and Tuscaloosa nonwork trips are 40, 64, and 77 percent respectively. Since these percentages apply only to those trips that started cold, cold-mode percentage for all trips can be obtained by multiplying the above cold-mode percentages by the percentage of all trips that started cold. The percentages are as follows for the cold-mode trips:

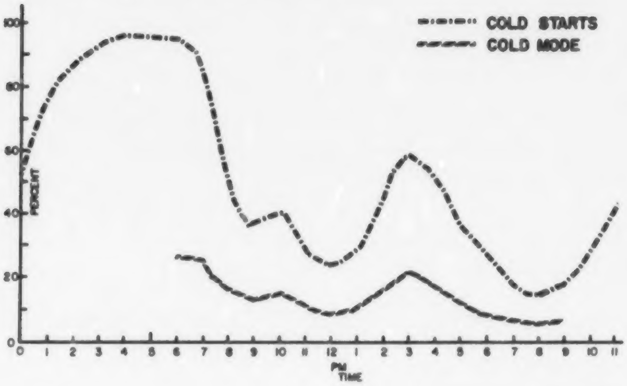
City	Work Trips	Nonwork Trips
Tuscaloosa	64 × 35 = 22	77 × 35 = 27
Birmingham	27 × 46 = 12	40 × 46 = 18

It is apparent that in the smaller city a higher percentage of trips will operate in the cold mode than in the larger city. These results apply to daily trip totals and will contain large uncertainties because of hourly changes in trip distribution, cold-start percentages, and temperatures. Therefore, such percentages can be considered only as gross approximations. A more accurate analysis will require that these variables be considered on an hourly basis as follows.

Suppose that, between 7 and 8 a.m. in Tuscaloosa, the typical January temperature is 35 F (1.7 C), the cold-start percentage is 78 percent, and 54 percent of all trips are work trips. The average trip duration is calculated as (0.54 × 13.13) + (0.46 × 10.88) = 12.10 min. All trips that start cold will operate 69.6 percent (8.42 ÷ 12.10) of the time in the cold mode. Therefore, all trips at this hour will operate 54 percent (0.78 × 0.696) of the time in the cold mode. Figure 6 shows the results of applying this technique to Birmingham between the hour beginning at 6 a.m. and the hour beginning at 9 p.m. The percentages of work trips and nonwork trips were obtained from analyses of screenline checks made between 6 a.m. and 10 p.m. Trip duration data were taken from trip distribution reports.

The above analysis is not intended to be an estimate of real-world conditions but to illustrate the importance of the cold-start correction, in particular, and of the trip-making process in general. Furthermore, it is important to study the cold-hot condi-

Figure 6. Cold mode profile for Birmingham.



tion not only in temporal detail but in spatial detail also. This spatial detail can be obtained by deriving the cold-hot profile from the origin-destination survey data on a zonal basis. The temporal distribution of trip purposes also needs to be studied. The origin-destination data contain a wealth of information that can and should be applied to air quality modeling.

AUTOMATING COMPUTATIONS IN PUBLICATION AP-42

The latest revision of the EPA emissions manual (4) is much more involved than earlier revisions. In general, it follows other revisions in its approach to the problem of calculating emissions, i.e., emission ratings for the various model years and the various vehicle types are combined to yield calendar year emission factors that can be applied to traffic on a roadway segment or network. However, a number of matters are considered either for the first time or in more detail than before. Such considerations include cold starts, ambient temperature, speed correction, and deterioration factors. Procedures for calculation of model-year mix are the same as before. The effect of these considerations is to greatly reduce the uncertainties inherent in the estimation of emission factors, but at the expense of the time involved, to say nothing of the multiple opportunities for errors. The reaction of the typical conscientious user will probably take one of two paths: He or she will either make a laborious effort to follow the procedures outlined or throw up his or her hands in despair and fall back on the average emission factors listed at the end of Publication AP-42. However, a third alternative is automating the computations recommended in Publication AP-42; this is the path that Alabama is investigating. The procedures of the document are so involved that the development of such a program requires a major effort, although one that we believe will pay for itself many times over in time saved. Alabama plans to release a preliminary review version of its documentation so that a thorough review can be made by EPA, the Federal Highway Administration, the Transportation Research Board, and any others who are interested. Wherever possible, the program will contain default values for those who do not have local data, such as national model-year mix data. (We plan to derive model-year mix for each county in Alabama and for the state as a whole from a program now under development using license plate registration data.)

In the automation, a technique for manipulating hourly variations in traffic is as follows. On a given roadway at a particular hour of the day, the contribution of traffic in grams per mile is a function of the emission factor representing that traffic corrected for all factors subject to hourly variations. Such hourly variations are traffic, ambient temperature, cold-hot operation correction, and speed correction. If all these variable quantities are known, then all the corrections can be calculated and combined (multiplied) at each hour to yield a total correction for that hour. Next, the correction factors for all 24 hours can be added, then multiplied by the uncorrected emission factor. The end result represents a daily (24-hour) emission factor for a particular roadway type or segment. This daily emission factor, after appropriate correction for model-year mix, can be used in a daily emission inventory model such as GRIDSUM and will implicitly contain the hourly variations noted. For an hourly emission factor, the product of all correction factors for that hour is multiplied by the uncorrected emission factor.

CONCLUSIONS AND RECOMMENDATIONS

1. Coordination between model developers and model users should be improved.
2. Additional automation is required to facilitate the use of models, particularly with respect to generating input for the models.
3. The APRAC-1A model needs to be revised, with particular attention given to emission factors.
4. The trip-making process requires additional analysis to determine the effects of cold starts on emissions, and these effects need to be incorporated into the models.

ACKNOWLEDGMENTS

The author wishes to express his thanks to the following colleagues: R. T. McNider of the Alabama Air Pollution Control Commission for his advice and assistance; W. T. Camps of the Alabama Highway Department for his outstanding work in analysis and programming; and Harris Cooper of the Alabama Highway Department for his help in the analysis of the trip-making process.

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SELECTED OBSERVATIONS ON MESOSCALE MODELING

Walter F. Dabberdt, Atmospheric Sciences Laboratory, Stanford Research Institute, Menlo Park, California

Before discussing the subject, I feel first obliged to define a mesoscale simulation model for inert pollutants. For simplicity, consider only carbon monoxide and assume virtually all emissions are from mobile sources. First, the model should prescribe the location and intensity of emission sources and their time variation. Second, atmospheric transport and diffusion must be treated. Third, receptor locations must be prescribed and representative CO concentrations computed. In the latter lies the difficulty: What constitutes a representative mesoscale pollutant concentration?

Qualitatively, the mesoscale is synonymous with the "neighborhood" scale; EPA (1) considers pollutant levels on this scale to be "representative of those areas of uniform land use . . . in which a captive population . . . is exposed." For large metropolitan areas, a concentration representative of average CO levels over an area of 1 km^2 and larger is a reasonable if arbitrary definition of the mesoscale. Other areas with relatively small urban cores may require a reduction in the representative mesoscale. The microscale generally ranges from 10 m to the lower limit of the mesoscale. (What is representative from the perspective of spatial scale may be compounded by complexities when an attempt is made to reconcile length and time scales; however, this problem is usually more germane to microscale analyses.)

In addition to providing area-average concentrations, mesoscale models should also provide some indication of the peak value or variance. To do this, the mesoscale model must also be able to simulate microscale dispersion phenomena such as those that occur near freeways or in street canyons. The microscale capability is particularly important when mesoscale model predictions are compared with observational data. Observational data are most often obtained from stations located to measure only hot-spot concentrations. Only with the use of a model able to accommodate microscale and mesoscale (2-tiered) phenomena can the areawide significance of observational data be properly interpreted.

OBJECTIVES OF MESOSCALE MODELING

Mesoscale (and microscale) modeling has 3 objectives:

1. Prediction of the absolute pollutant concentration attributable to a specific emission source;
2. Prediction of relative changes in pollutant concentrations from changes in emission rates or meteorological conditions; and
3. Combination of the first and second objectives.

Interestingly enough, most applications of mesoscale models fall into the second category, yet most (if not all) model-evaluation studies are of the first kind. In view of the large relative changes in vehicular CO emission rates and the long-term data records now available in some cities, it would be particularly beneficial to test the performance of mesoscale models in simulating such changes.

PURPOSES OF MESOSCALE MODELING

Another way to consider mesoscale models is by the specific purposes to which they may be put. Three such purposes stand out:

1. Short-term forecasting;
2. Impact assessment of new emission sources; and
3. Impact assessment of changes to existing emission sources.

The first purpose is sufficiently restrictive that it would appear to apply only to emergency episode conditions. (The Fairbanks, Alaska, air quality control region is the only area in the United States likely to ever encounter episodic CO concentrations.)

Impact assessment of new emission sources is pending in the form of the proposed indirect source and parking management regulations. At first glance, the indirect source and parking regulations appear to be restricted to the microscale because the local CO concentration induced by the facility must be compared with the national ambient air quality standards. Yet this comparison has to include existing "background" (i.e., mesoscale) concentrations. Furthermore, the 8-hour ambient standard is more likely to be jeopardized than the 1-hour standard; on the 8-hour time frame, mesoscale concentrations are likely to be significantly greater than the local CO contribution by the facility under review.

Impact assessment of changes to existing emission sources is particularly important, as in the preparation of air quality maintenance plans. Here, mesoscale models have to predict changes in areawide CO levels that might result from combinations of changes in vehicle volumes, speeds, and emission rates.

MODEL EMPHASIS AND IMPROVEMENTS

Special attention should be devoted to the evaluation and improvement of mesoscale CO models for the simulation of 8-hour concentrations. In addition, specific attention should be given to improvements in model versatility and resolution in the following areas.

1. Meteorology. There should be enhanced representation of the near-surface wind field, through input of stream lines or trajectories or of a receptor-oriented wind vector, as examples. The vertical dispersion coefficient should be specified on the basis of surface characteristics (e.g., land use, topography).
2. Emission rates. Mesoscale models should include the latest EPA factors for hot and cold start ratio, altitude, temperature, and so forth. Microscale submodels should ideally include emissions by operating mode (i.e., idle, acceleration-deceleration, and cruise) and location on the roadway link.
3. Traffic data. Better speed and volume resolution should be incorporated, particularly in the urban core where low speeds (under 24 km/h) occur.
4. Microscale submodels. Dispersion routines should be available for simulation from a number of common roadway configurations: at-grade roadway, cut section, fill section, and viaduct.

One last improvement to most models that could (and should) be made immediately is better user documentation. Improved user manuals should include a summary of the model formulation, assumptions, and limitations; program listing; input data coding forms; user notes; and complete applications.

COSTS AS A CONSTRAINT

Most mesoscale CO models are relatively inexpensive to operate in terms of computer dollars. This is particularly true when these costs are weighed against the total cost of acquiring and encoding the meteorological and emission data and of evaluating the performance of the model against monitoring data. However, cost is a major factor when poor meteorological or traffic input data are used. When such data are used, the computational exercise becomes an end in itself providing worthless output. The real net cost is then measured in terms of either the human health and welfare endangered or the unnecessary and inconvenient controls imposed because of an incorrect assessment.

REFERENCE

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SAPOLLUT: ESTIMATING THE AIR QUALITY IMPACT OF VEHICULAR EMISSIONS RESULTING FROM A TRAFFIC ASSIGNMENT

Thomas P. Kozlowski, Federal Highway Administration

Special area pollution (SAPOLLUT) is the noise and air quality analysis portion of special area analysis (SAA) developed by the U.S. Department of Transportation. SAA is an attempt to encourage the consideration of social and environmental factors in the planning of transportation systems for urban areas by providing the analytical tools to address some of the social and environmental issues. SAA was initially included as a mandatory item of the 1974 National Transportation Study for all urban areas greater than 500,000 population. Participation in the SAA portion of the study was later made voluntary.

The purpose of the air quality analysis section of SAA is to present a methodology to quantitatively estimate the daily atmospheric loading of the highway-related pollutants (carbon monoxide, hydrocarbons, and nitrogen oxides) resulting from the daily travel on an urban street and highway system. This analysis is pertinent due to the requirements of the Clean Air Act Amendments of 1970 and the Federal-Aid Highway Act of 1970. Consequently, SAPOLLUT is being used in many areas for transportation system alternatives evaluation and transportation and air quality consistency determinations.

Approximately 50 copies of the program software have been distributed by the Urban Planning Division of the Federal Highway Administration to state transportation and highway departments, local urban transportation planning agencies, air quality planning agencies, consultants, and universities. SAPOLLUT was initially distributed in late 1973. Many comments on the program were received and, as a result, a new version of the program was developed. Major changes to the program have been made that improve its operating efficiency, add flexibility to the input requirements, and increase the output options. I will discuss these changes later, but first I will describe the basic SAPOLLUT methodology, program operation, data requirements, and output.

SAPOLLUT METHODOLOGY AND PROGRAM OPERATION

SAPOLLUT is an emission program; that is, the measure of the air quality impact is in kilograms of pollutants. The total amount of pollutants may be, at the user's option, stratified by hour of day, area type, functional classification, and pollution district.

A standard Federal Highway Administration (FHWA) historical record and default values supplied internally in the program (or user-specified values) are used to stratify the volume on each link in the network (except controid connectors) by a battery of factors according to the functional classification and area type of the link. The vehicle miles of travel (VMT) is also factored for 3 vehicle types and by model year for each type. The model year of interest and the previous 13 model years are used.

For the required emission factors, the program enters an internal table of carbon monoxide, hydrocarbons, and nitrogen oxide exhaust emission factors, deterioration factors, speed adjustment factors, and hydrocarbon evaporative emission factors. These 126 factors (3 pollutants × 3 vehicle types × 14 model years) are multiplied by the factored link VMT to give the hourly carbon monoxide, hydrocarbon, and nitrogen oxide emissions on each link for each hour. The new version of SAPOLLUT does not actually go through each of these steps for each link; it combines the tables where possible prior to network processing to optimize the link processing. This has resulted in a substantial decrease in CPU time required over the original SAPOLLUT.

The program will also estimate exhaust emissions from intrazonal travel if the necessary data are input. These are the percentage of the total travel in a zone not represented on the network and an arbitrary speed for this local travel.

A more detailed discussion of the SAPOLLUT methodology is given in another report (11).

DATA REQUIREMENTS AND OUTPUT

A loaded historical record is all that is necessary to use SAPOLLUT. Each link of the network must have coded average daily traffic (ADT); length; area designation (CBD, central city, suburbs); functional classification (freeway, arterial); and capacity or speed table stratified by hour, functional classification, and area type. As mentioned earlier, SAPOLLUT contains default tables that are used to factor the ADT into hourly, directional, and vehicular volumes. These tables are also used to determine the link speed and emission factors. The tables used in SAPOLLUT are

1. Hourly distribution of ADT,
2. Hourly distribution of directional split,
3. Hourly truck factors,
4. Speed versus volume to capacity ratio,
5. Distribution of age of vehicles,
6. Exhaust emission factors (CO, HC, NO_x),
7. Evaporative hydrocarbon factors,
8. Emission deterioration factors, and
9. Emission adjustment due to speed.

These tables were derived from national studies, and the tables for computing the emission factors are taken from the EPA publication (12); various reports (1, 2, 3, 4, 5, 6, 7, 8) are the sources of information for these tables. A draft report by the SAE Task Force on Emission Projection Techniques was also a source.

I would like to emphasize that the software has been designed to allow for easy user input of location-specific data whenever possible. We strongly encourage using local data when they are available. The user also has the option to redefine the location of the variables on the input historical record. This option is useful when a standard FHWA format historical record is not used.

The output of SAPOLLUT is a series of tables that give the amount of hydrocarbons, carbon monoxide, and nitrogen oxide (in kilograms) emitted by hour, or a range of hours, for a specific area type and functional classification. The vehicle miles of travel for each hour is also given along with the ratios of grams of pollutant per vehicle mile and grams of pollutant per passenger mile (Figure 1). The amount of pollutants in specific "pollution districts" may also be computed and output on a daily basis for freeways and arterials only.

EXPERIENCE WITH SAPOLLUT

Many people have shown a great deal of interest in SAPOLLUT, and, as a result, we were able to get some good feedback on its use. It soon became obvious where the strengths and weaknesses in the program were.

Since SAPOLLUT interfaces directly with the Federal Highway Administration's urban transportation planning computer programs, it was the obvious choice as the next step in evaluating the air quality impact of the transportation system. This interfacing,

Figure 1. SAPOLLUT output.

```
AREA-1 CBD
FUNC-1 FREEWAY

              VEHICLE       KILOGRAMS OF AIR POLLUTANT          POLLUTANT  (GRAMS/VEH-MILE)         POLLUTANT  (GRAMS/PASS-MILE)
HOUR           MILES      (1)=CO     (2)=NO     (3)=HC       (1)=CO     (2)=NO     (3)=HC       (1)=CO     (2)=NO     (3)=HC
----          -------     ------     ------     ------       ------     ------     ------       ------     ------     ------

  0              255       1.069      1.797       .232        4.193      7.052      0.910        2.092      3.526      0.455
  1              137        .727      1.656       .151        5.456     10.630      1.124        2.728      5.315      0.562
  2               85       0.524      1.392       .127        6.159     16.388      1.260        3.085      8.194      0.630
  3               45       0.450      1.234      0.096        5.234     15.705      1.130        2.649      7.853      0.565
  4              173       1.292      2.763       .252        7.035     16.263      1.483        3.902      8.132      0.742
  5              343       2.122      3.345       .422        6.245      9.668      1.236        3.123      4.834      0.618
  6              934       7.101      4.353      1.241        7.696      4.659      1.328        3.848      2.329      0.664
  7            1.444      14.154      4.252      2.225        9.667      2.943      1.541        4.984      1.472      0.770
  8            1.143      12.457      3.442      1.042       10.454      3.748      1.633        5.227      1.674      0.816
  9              765       5.735      3.144      1.117        7.352      4.118      1.464        4.176      2.059      0.732
 10              682       4.373      2.876       .716        7.327      4.232      1.368        3.663      2.116      0.674
 11              765       5.529      3.177      1.054        7.621      4.156      1.379        3.812      2.078      0.689
 12              765       5.813      3.123      1.026        7.366      4.085      1.342        3.683      2.043      0.671
 13              765       5.714      3.120      1.047        7.536      4.095      1.370        3.783      2.046      0.685
 14              836       7.815      3.335      1.121        8.223      3.572      1.414        4.102      1.786      0.707
 15            1.274      12.888      4.060      2.011       10.115      3.186      1.578        5.057      1.593      0.789
 16            1.614      15.101      4.369      2.461        9.376      2.706      1.525        4.988      1.353      0.762
 17            1.358      11.116      3.335      1.921        8.173      2.454      1.325        4.089      1.227      0.663
 18              845       4.676      2.613       .925        5.550      3.042      1.094        2.930      1.541      0.547
 19              682       3.122      2.293       .641        4.574      3.366      0.943        2.297      1.680      0.472
 20              535       2.562      2.218       .541        4.529      3.732      0.908        2.154      1.865      0.454
 21              517       2.427      2.061       .493        4.762      4.342      0.973        2.381      2.021      0.490
 22              425       1.548      2.135       .346        3.645      5.027      0.815        1.822      2.513      0.407
 23              342       1.285      1.737       .285        3.782      5.112      0.839        1.891      2.556      0.419
----          -------     ------     ------     ------       ------     ------     ------       ------     ------     ------
TOT           16.783     132.657     64.567     22.752        7.911      4.036      1.336        3.905      2.018      0.668
```

Figure 2. Example of SAPLSM link report.

```
21APR75  14.50.03           SAPULSUM REPORT  1

----LINK---  HOUR ----  GRAMS OF POLLUTANTS ----  LINK    DAILY  DAILY
ANODE BNODE                CO        NOX      HC   KM.  VEH KM.  VOLUME


  31    32  0-23        8547       5893    1623  0.22    1386    6300

  32    33  0-23       14034       7376    2449  0.21    1469    8900

  33    74  0-23       14833       5691    2578  0.24    2184    9100

  33    34  0-23       12349       6222    2128  0.15    1590   10600

  33    80  0-23        9354       4027    1526  0.10    1060   10600

  34   108  0-23        5156       1569     757  0.17     442    2600

  34    35  0-23       33290      15476    5568  0.34    4012   11800

  35    48  0-23       56896      12533    7991  0.30    5070   16900

  35    36  0-23       29497      11161    4527  0.16    2896   18100

  35    49  0-23       13010       9696    2442  0.17    2142   12600

  36    37  0-23       32957       6556    4489  0.16    2720   17000

  37    95  0-23        7774       1479    1046  0.14     616    4400

  37    38  0-23       33669       6777    4606  0.17    2805   16500

  37    94  0-23        4902       1573     781  0.15     525    3500

  38   101  0-23       19866       3942    2647  0.11    1650   15000

  40   101  0-23        7187       2837    1140  0.05     755   15100

  41    42  0-23       18925       8015    3040  0.15    2070   13800

  41    71  0-23        4194       2818     784  0.09     666    7400

  42    43  0-23       15405       5584    2379  0.11    1518   13800

  43   107  0-23       11051       2016    1474  0.25     850    3400

  46    78  0-23        2175       1127     429  0.52     416     800

  46    47  0-23       12813       5832    2402  0.44    2200    5000

  47    61  0-23       13307       4419    2186  0.16    1728   10800

  47    48  0-23       21899       4355    2984  0.11    1804   16400
```

without any data adjustments, we believe is one of its strongest attributes. SAPOLLUT also recognizes the different transportation and air quality factors that must be accounted for in any transportation-air quality analysis. Vehicle type, vehicle age, facility type, area type, speed, and VMT are all addressed in computing the amount of pollutants emitted.

Some of the major drawbacks in SAPOLLUT centered around its extensive computation time and its rigorous requirements for the input data. We also received several comments on its inability to diffuse pollutants.

THE NEW SAPOLLUT

SAPOLLUT was originally developed as a user-oriented program. The data needed to run the program were in general easily obtainable, and the user had many options on the degree of refinement of the analysis. Several shortcomings of the program had to be corrected, however, to make it truly user oriented.

The computation time was by far the biggest problem. Several agencies had to shut down the program after it ran for a couple of hours, wasting several hundreds of dollars. The new version of SAPOLLUT has corrected this problem by first summing the emission tables for each vehicle type and pollutant type prior to link processing. This technique has resulted in a substantial savings of CPU time. With data from the Puget Sound area, I obtained an 89 percent reduction in CPU time between the old and new versions (23 versus 2.5 min).

Most of the factors used in SAPOLLUT are a function of the area type and functional classification of the link. Consequently, both bits of information are needed to process each link. This has presented a problem for some users since the area type and functional classification were not coded for each link. This meant that they had to go back and code this information on each link card, a tedious task. The new program still requires functional classification and area type information for each link, but the user now has greater flexibility in specifying links of certain functional classification or area type or both to be processed. A fourth area type has also been added.

Another major modification to SAPOLLUT has been the addition of a SELECT option. This allows the user to select only certain hours or ranges of hours or portions of the network or all of these for processing. The original program did not allow for more than one range of hours or for certain links to be specified. This option greatly enhances the versatility of SAPOLLUT for use in either peak-hour analyses or route analyses.

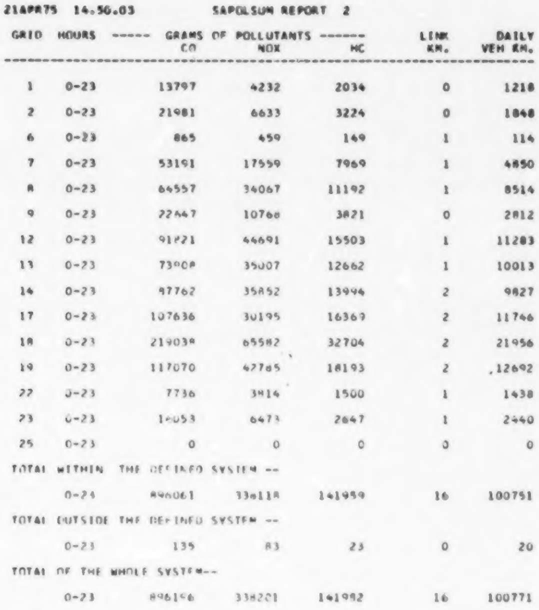
SAPOLLUT now has the capability to "window in" on a rectangular area. The user just has to specify the x and y coordinates of the corners.

As mentioned earlier, SAPOLLUT is an emission program. It does not diffuse and consequently its output cannot be directly related to a concentration standard. The APRAC-1A urban diffusion model computer program has been modified to accept the output of the SAPOLLUT program. This will enable users of the SAPOLLUT-APRACMOD package to compute emissions for hydrocarbons, carbon monoxide, and nitrogen oxide and to get concentrations of carbon monoxide. Another major concern of many users was the output format of SAPOLLUT. A spatial stratification by link, zone, or grid or all of these was requested. We too felt a need for this type of output, and consequently a new post processor program was developed.

SAPLSM

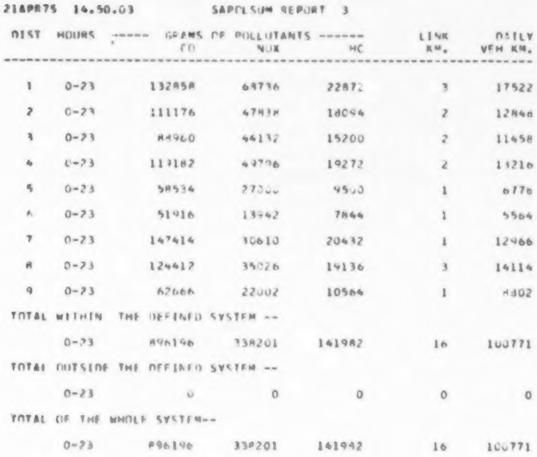
SAPLSM, the SAPOLLUT post processor program, summarizes the link emissions by link, zone (districts), and grid. The program reports also contain the link distance and VMT information. The user has complete flexibility in specifying the grid system and range of hours. Examples of the reports are given in Figures 2, 3, and 4. The original output of SAPOLLUT has been kept in the SAPOLLUT program. SAPLSM merely reads an output file from SAPOLLUT and outputs it in the user-specified form.

Figure 3. Example of SAPLSM grid report.



```
21APR75  14.50.03              SAPOLSUM REPORT  2

GRID  HOURS  -----  GRAMS OF POLLUTANTS ------         LINK      DAILY
                        CO         NOX         HC       KM.    VEH KM.
-----------------------------------------------------------------------

   1   0-23          13797        4232       2034         0       1218

   2   0-23          21981        6633       3224         0       1848

   6   0-23            865         459        149         1        114

   7   0-23          53191       17559       7969         1       4850

   8   0-23          64557       34067      11192         1       8514

   9   0-23          22847       10768       3821         0       2812

  12   0-23          91821       44691      15503         1      11283

  13   0-23          73908       35007      12662         1      10013

  14   0-23          97762       35852      13994         2       9827

  17   0-23         107636       30195      16369         2      11746

  18   0-23         219038       65582      32704         2      21956

  19   0-23         117070       42785      18193         2     ,12692

  22   0-23           7736        3814       1500         1       1438

  23   0-23          16053        6473       2847         1       2440

  25   0-23              0           0          0         0          0

TOTAL WITHIN  THE DEFINED SYSTEM --

       0-23         896061      338118     141959        16     100751

TOTAL OUTSIDE THE DEFINED SYSTEM --

       0-23            135          83         23         0         20

TOTAL OF THE WHOLE SYSTEM--

       0-23         896196      338201     141982        16     100771
```

Figure 4. Example of SAPLSM district report.



```
21APR75  14.50.03              SAPOLSUM REPORT  3

DIST  HOURS  -----  GRAMS OF POLLUTANTS ------         LINK      DAILY
                        CO         NOX         HC       KM.    VEH KM.
-----------------------------------------------------------------------

   1   0-23         132858       69736      22872         3      17522

   2   0-23         111176       47838      18094         2      12848

   3   0-23          84960       44132      15200         2      11458

   4   0-23         113182       49796      19272         2      13216

   5   0-23          58534       27300       9500         1       6776

   6   0-23          51916       13942       7844         1       5564

   7   0-23         147414       30610      20432         1      12966

   8   0-23         124412       35026      19136         3      14114

   9   0-23          62666       22002      10564         1       8802

TOTAL WITHIN  THE DEFINED SYSTEM --

       0-23         896196      338201     141982        16     100771

TOTAL OUTSIDE THE DEFINED SYSTEM --

       0-23              0           0          0         0          0

TOTAL OF THE WHOLE SYSTEM--

       0-23         896196      338201     141982        16     100771
```

The decision to develop a new program for this task was based on economy of operation. Only one run of SAPOLLUT is now needed. The user has the option either to input the results into APRACMOD or to summarize them by using SAPLSM. The user may at a later time get a different summary or rerun APRACMOD without having to run SAPOLLUT again.

COLD STARTS

One of the major objectives in developing a new version of SAPOLLUT was to incorporate a method of calculating emissions due to cold starts. Cold-start emissions are a function of the number of trips made and not the length of the trip as are hot-running emissions. This presented us with somewhat of a problem in developing a methodology that accounts for both types of emissions and uses the transportation data that are generally available.

We opted to relate the land use of the traffic analysis zone to the hourly trip origins in that zone. A cold-start emission rate (in grams/trip) can then be applied to this volume. A hot-running emission rate (in grams/mile) can be applied to the interzonal volumes.

This was accomplished by developing a series of tables that relate land use to an hourly factor of trip origins. This hourly factor is further stratified by the parking duration. This information was developed by analyzing several sets of internal trip report cards. The parking systems analysis (10) procedure was used for this analysis.

The cold-start emission rates were computed by applying the cold-start ratio developed by Cirillo and Wolsko (9) to the emission factors of Publication AP-42 (8). The hot-running emission rates were also developed in a similar manner as described by Cirillo and Wolsko. The cold-start analysis in SAPOLLUT only applies to light-duty vehicles and carbon monoxide and hydrocarbons. The default emission tables are taken directly from Publication AP-42 and consequently the user has to revise them to strictly hot-running emissions if the COLDSTART option is used.

Nine land use categories are used in this analysis: residential, commercial, offices, industrial, agricultural, public utilities, institutional, recreational, and undeveloped. A land use classification must be coded for each centroid connector. As with all default tables in SAPOLLUT, it is strongly recommended that locally developed data be used whenever possible.

SUMMARY

SAPOLLUT is an effective tool to estimate the air quality impact of a highway system. The easily obtainable input data and extensive user options have made SAPOLLUT applicable to most systemwide transportation-air quality analyses.

Extensive modifications to SAPOLLUT have improved its operating efficiency, added flexibility to its input requirements, and increased the analysis options. A post processor program, SAPLSM, was developed to summarize the emissions by either link, zone (district), or grid. The APRAC-1A urban diffusion model computer program has been modified to accept the output of SAPOLLUT.

These modifications were developed with the help of the many SAPOLLUT users, and we hope to have their continued support in the future.

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USER EXPERIENCE WITH SAPOLLUT

Carlton T. Nash, Environmental Quality Division, Virginia Department of Highways and Transportation

In this paper, I will discuss 2 different aspects of the transportation and air quality relation at the regional level: first, experience that the Virginia Department of Highways and Transportation has had in using the SAPOLLUT air quality analysis emission program and second the adequacy of this approach in relating to the impacts of proposed transportation plans and programs on air quality.

The Federal Highway Administration manual (1) requires that land use planning, transportation planning, and air quality planning be coordinated annually through the local planning agency, the Virginia Department of Highways and Transportation, and the Virginia Air Pollution Control Board. Coordination and consistency determinations of the transportation plans and programs with the state implementation plan in most cases can only occur after a technical analysis has been performed that assesses the air quality impacts of the regional transportation network. Proposed improvements to the existing transportation network are called the urban transportation plans and programs.

The technical analysis used by the Virginia Department of Highways and Transportation in most of the major urban areas was the air quality analysis emissions program (SAPOLLUT) of the Federal Highway Administration manual (2) of August 1973. Other technical analyses and discussions assessing regional impacts resulted from consultation with the Virginia Air Pollution Control Board and the U.S. Environmental Protection Agency.

Of the 7 major urban areas in Virginia, a complete SAPOLLUT analysis was performed for only 5. A partial analysis was performed for 1 area, which is undergoing a level 2 review. The other area, northern Virginia, was studied by the Metropolitan Washington Council of Governments and underwent intensive examination with a regional carbon monoxide model as well as a total emission analysis.

In these areas where the complete SAPOLLUT analysis was carried out, emissions in kilograms per day were calculated for the 3 major transportation-related pollutants: carbon monoxide, hydrocarbons, and nitrogen oxides. Emissions were calculated for 3 functional types of highway facilities: freeways, arterials, and local streets. Finally, emissions for each pollutant and for each functional type of facility were calculated according to their location in the central business district, central city, and the suburb area of the study region.

A complete SAPOLLUT analysis was carried out for a base year in which most recent socioeconomic data had been used to verify transportation models. The target year for the transportation plans and programs was studied by assuming both target-year traffic on a completed target-year transportation system and target-year traffic on the base-year transportation system. An interim year was studied through interpolation of base-year and target-year vehicle miles of travel and by applying interim-year emission factors. The attainment year for the national ambient air quality standards, 1975, was chosen for the interim year.

Results of these analyses were incorporated into a report that also characterized the nature of transportation and air quality within not only the transportation study area but also the air quality control region. A description of the plans and programs was presented as well as their location. The report also discussed the transportation models and their calibrations and prediction techniques. Air quality information for each pollutant such as the priority status, air quality maintenance status, and the maximum recorded concentrations specified in the state implementation plan was presented. In general terms, the interrelation of climatological, meteorological, and topographical parameters was related to the air quality of each region. Finally, the report summarized the models used in the analysis, the emission factors, and the methodologies used in assessing the air quality impacts of transportation systems.

The conclusions contained a consistency determination for the proposed plans and programs for each pollutant, thereby describing the consistency of the urban transportation plans and programs with the state implementation plan. The report also outlined the consultation that had occurred between the planning agencies, the Department of Highways and Transportation, and the Virginia Air Pollution Control Board in developing adequate technical procedures.

The major advantage of the SAPOLLUT methodology is that it allows pollutant emissions from various transportation alternatives to be compared by using an established data bank of transportation information. Furthermore, it could be used to determine whether changes in a transportation network will cause a change in the spatial distribution of pollutant emissions. Operationally, the SAPOLLUT procedures are fairly easy to incorporate and apply.

One of the most obvious shortcomings of the SAPOLLUT model is that the output results are expressed as total emissions in unit mass whereas the designated national ambient air quality standards are expressed as a concentration in micrograms per cubic meter. Therefore, no direct comparison of the air quality impact of the transportation network to the national standards could be made.

That portion of the output data that is most closely scrutinized is hydrocarbon emissions. Calculation of reductions in emissions between a base year and future years allows for comparison between values specified in the state implementation plan and reductions caused by alternate plans and programs. The results cannot be used to directly determine the magnitude, the location, or the quantity of violations of standards.

The resolution of the carbon monoxide information is not adequate within the central city, central business district, or suburb to allow identification of impacted sites or quantification for comparison with standards. This problem will be partially resolved when the SAPOLLUT model is linked to the APRAC-1A model. However, it may be most appropriate to simply identify potential hot spots at the systems level and then quantify their concentrations at the project level.

Nitrogen oxides are reactive in nature and cannot be estimated through use of the SAPOLLUT emission model. Furthermore, emissions are in total nitrogen oxides, and the national standard, an annual standard, is for nitrogen dioxide only. In addition, the results, like those for hydrocarbons, are in emission units and not in concentrations.

SAPOLLUT is basically a computerization of the Environmental Protection Agency emission factors. It interfaces transportation planning and air quality planning by using as input data from the standard FHWA urban transportation planning computer programs. The reliability of the results is, therefore, dependent on the accuracy of the input data as well as the emission factors.

The accuracy of the transportation data used as a basis for calculating air quality impacts lacks the required preciseness to be fully dependable. The level of sophistication of transportation planning procedures required by the air quality planning process falls short of being reliable enough to be used with confidence as a basis for calculations whose results will be compared to exact standards. Some consideration must be given to the deficiencies of a process calculating figures that are often held as impeccable. Application of the SAPOLLUT methodology is more appropriate for comparison of alternatives to one another than comparison of alternatives to absolute standards. Otherwise, more detailed information for a particular region should be obtained for directional split, percentage of heavy-duty vehicles, speeds, percentage of ADT by hour, and so on.

New emission factors will soon be officially released by the Environmental Protection Agency. These factors were developed for a complete vehicle trip and not specifically for vehicles on a particular highway link. Furthermore, the emission factors are valid only for vehicle speeds up to 45 mph (72 km/h). Taking the emission factor at 45 mph and using it for 45 to 55 mph (88 km/h) give conservative results. The combined effect of these 2 considerations could yield results that in some cases are significantly conservative. In addition, detailed information for 6 different vehicle types should be used for an accurate analysis with these emission factors. Such information is expensive and difficult to obtain with any reliance.

One application problem was specifically experienced by the Virginia Department of Highways and Transportation. The department was not able to use the capacity restraint process as suggested by special area analysis because of the operational computer expense and lack of detailed capacity information on the entire transportation network. Therefore, the department had to use the free assignment with network speeds.

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MOBILE SOURCE EMISSION FACTORS: STATE OF THE ART AND FUTURE PROGRAMS

Marcia E. Williams, Office of Mobile Source Air Pollution Control, U.S. Environmental Protection Agency, Ann Arbor, Michigan

Various approaches to air quality modeling have been used to relate changes in emission rates to changes in ambient air quality. The commonly used rollback model assumes that a change in the amount of pollutant emitted from one or more source categories will result in a directly proportional change in ambient air quality. The model does not consider the localized effects of meteorological and topographical conditions nor does it allow for changes in background pollutant concentration and emission distribution in space and time over the projection period. Moreover, point source indicators of air quality may not be representative of air quality over an entire region of modeling interest. The use of the second highest concentration value as a base predictor may compound this problem since limited data analyses indicate that it may not be the best predictor of average mean ambient concentration or number of times the standard is exceeded annually either at a single sampling point or in a region (1).

Diffusion models, although considerably more data intensive than the simple proportional model, can be expected to improve predictive ability since they recognize the importance of meteorological and topographical variables. However, all models are limited by the accuracy of the input data. Before a model can be applied, an estimate of the amount of pollutant emitted must be computed for the base year and the future years of interest. The amount of pollutant emitted for future years is a function of both the emission factor, defined as the rate at which a pollutant is released to the atmosphere as a result of some activity, and the growth rate of the activity. In addition, accurate estimates of base-year ambient concentration and, in the case of diffusion models, meteorological and topographical variables are needed. This paper will address the sources and accuracy of the emission factor inputs necessary to perform air quality modeling of carbon monoxide.

Carbon monoxide is largely a localized problem although a second-order areawide problem may exist as a result of workday buildup of CO. Moving a monitor a few feet will usually result in a large change in measured concentration, and locating monitors in different places within a central business district will show large concentration differences (1). High CO concentrations are normally found at busy intersections, streetside, and other locations of high traffic density. As a result of the hot-spot nature of CO, motor vehicles tend to dominate the modeling situation and stationary sources have little impact.

Estimates contained in the National Emissions Data System (NEDS) indicate that during 1973 more than 93 million tons (84.4 Tg) of CO were emitted in the United States by man-made sources. Seventy-eight percent of these are attributed to mobile sources, and the automobile alone accounts for nearly 50 percent. Most urban monitoring sites at which ambient CO concentrations are high are located in areas of high traffic density and are rarely influenced by stationary sources of CO. Urban violations of the national ambient air quality standard for CO are almost exclusively due to vehicular traffic, and the importance of stationary sources is even less than indicated by the nationwide emissions.

Estimates for 1971-1974 calendar year stationary source contributions to hot-spot problems are on the order of 3 percent. Although further control of mobile source CO can be expected to increase the importance of an accurate determination for stationary source emission factors and growth rates, the overriding concern at present is in the area of mobile source emission factors. Any comparison of the effectiveness of alternative control strategies for achieving ambient air quality improvement or the need to evaluate the implications of new or existing indirect sources is dependent on the ability to estimate the CO emission factor under various conditions.

EPA PROGRAM TO MEASURE MOBILE SOURCE EMISSION FACTORS

The Congress, through the enactment of the Clean Air Act of 1963 and amendments thereto, provided for a national air pollution program to monitor and control emissions from new motor vehicles. Administrative responsibility for the air pollution control program is vested with the U.S. Environmental Protection Agency (EPA). The first nationwide standards, together with the testing and certification procedures, were issued in 1966 and were applicable to 1968 model-year passenger vehicles and light-duty trucks sold within the United States. Levels for maximum allowable emissions were imposed initially on hydrocarbon (HC) and CO effluents only. Increasingly stringent standards have been introduced since the initial standards along with light-duty vehicle test procedure changes in 1972 and 1975. Heavy-duty vehicles were first subject to control in 1970, and motorcycles are first scheduled to be controlled in 1978. The current and projected CO standards by mobile source category are given in Table 1 along with the percentage of urban control achieved by each standard over the preemission control level. Best estimate future standards are included where known.

EPA has recognized that a realistic assessment of the effectiveness of federal air pollution regulations requires the measurement of emissions from production vehicles being driven by the public. This estimate of federal regulation effectiveness is necessary before states can assess their air quality attainment and maintenance plans. Whether vehicles meet emission standards throughout their lives depends on many items: owner maintenance practices, extent of tampering with the emission control system or emission sensitive parts, owner usage practices, failure of the manufacturer to adequately translate acceptable prototype design to mass production, poor assembly line quality control, and failure of prototype durability test to simulate real-life durability. To answer the question of how well vehicles perform in actual use, EPA has administered a series of exhaust emission surveillance programs. Test fleets of consumer-owned vehicles within various major cities were selected by model year, make, engine size, transmission, and carburetor in such proportion as to be representative of the normal production of each model year as well as the contribution of

Table 1. Current and projected CO emission standards by mobile source and control achieved.

Source	Year	Standard	Reduction (percent)
Light-duty vehicles	1975-1977 federal	15 g/mile	83
	1975-1977 California	9 g/mile	90
	1978 and later statutory	3.4 g/mile	96
	1978-1979 train recommendation	15 g/mile	83
	1978-1981 Ford recommendation	15 g/mile	83
	1980-1981 train recommendation	9 g/mile	90
	1982 and later train recommendation	3.4 g/mile	96
Light-duty trucks	1975-1977 federal	20 g/mile	77
	1976 and later California	17 g/mile	80
	1978 and later recommended federal	18 g/mile	79
Motorcycles	1978-1979 recommended federal	27 g/mile	21
	1980 and later recommended federal	3.4 g/mile	90
Heavy-duty trucks[a]	1975-1977 federal	40 g/hp-hr	32
	1975-197[illegible] California	30 g/hp-hr	38
	1977 and later California	25 g/hp-hr	41
	1977 and later recommended federal	25 g/hp-hr	41

Note: 1 g/mile = 0.6 g/km and 1 g/hp = 0.00134 g/W.

[a] Percentage reductions for heavy-duty gasoline trucks are given. CO levels for heavy-duty diesel trucks are considerably below standards.

that model year to total vehicle miles traveled. In the case of heavy-duty vehicles, fuel type and gross vehicle weight were also key items in the stratification scheme. A list of past and ongoing surveillance projects is given in Table 2.

The data collected in these programs are analyzed to provide mean emissions by model-year vehicle in each calendar year, change in emissions with the accumulation of mileage, change in emissions with the accumulation of age, percentage of vehicles complying with standards, and effect of vehicle parameters on emissions (engine displacement, vehicle weight). These surveillance data, along with prototype vehicle data, assembly line test data, and technical judgment, form the basis for the existing and projected mobile source emission factors presented in Publication AP-42 (2). All estimates of 1972 calendar-year emission factors are obtained directly from actual measurements in surveillance programs as are the projected deterioration rates for 1972 and earlier model-year vehicles.

The EPA emission factor surveillance program has paralleled or slightly preceded the EPA regulatory program. Such a situation is to be expected since the need to regulate usually is based on source-pollutant characterization. Both the emission factor program and the regulatory program depend on a valid test procedure over which emissions are measured. Test procedures are developed when regulation is anticipated.

It has been the intent of the EPA regulatory program to develop standards for a test procedure that represents urban emissions. Reductions during such a test procedure could be expected to predict reductions in actual urban emissions for area pollutants. For localized pollutants such as CO, the ability of the test procedure to predict changes in emissions depends on the similarity of the localized driving pattern and associated operating conditions to those in the test procedure. That is, it depends on the adequacy of the test procedure as a good yardstick for emission reduction. At the present time, EPA has 2 test procedures: one for light-duty vehicles (including cars, light trucks, and motorcycles) and one for heavy-duty vehicles.

The 1975 light-duty federal test procedure (FTP) measures emissions on a grams-per-mile (grams-per-kilometer) basis over a typical urban home-to-work trip. The actual test measures the emissions during 3 types of driving: a cold transient phase (representative of first 505 sec after vehicle start-up following a long engine-off period), a hot transient phase (representative of first 505 sec after vehicle start-up following a short engine-off period), and a stabilized phase (representative of warmed-up vehicle operation). The weighting factors used are 20, 27, and 53 percent of total miles (time) in each of the 3 phases respectively. These weighting factors can be viewed in 2 ways. On an areawide basis, the weighting factors imply that 43 percent (20/47) of vehicle trips start with the vehicle engine in a cold condition and 57 percent of vehicle trips start with the vehicle engine in a warm, but not stabilized, condition. On a localized basis, the weighting factors imply that 20 percent of the light-duty vehicles in the area of interest are operating in a cold condition, 27 percent are operating in a hot start-up condition, and 53 percent are operating in a hot stabilized condition.

The 1975 light-duty FTP requires that emission measurements be made within the limits of a relatively narrow temperature band (68 to 86 F or 20 to 30 C). The FTP has an average speed of 19.6 mph (31.4 km/h) with approximately 18 percent idle time and speeds as high as 57 mph (91.2 km/h). The test assumes the vehicle is loaded minimally (driver plus fuel only) and vehicle inertial weight and road-load horsepower are simulated for a level road condition. Air-conditioning is simulated by adding additional load.

The 1975 light-duty FTP is the standard test procedure used to test passenger cars, light-duty trucks, and motorcycles. The driving cycle attempts to simulate typical personal usage transportation in an urban environment. EPA has recognized that, although the FTP represents average urban operation, it may not represent specific localized conditions. Therefore, the emission factor surveillance programs have also collected data on vehicle operation at other than standard temperatures and other than standard loads. Modal emission data (idle, cruise, and acceleration and deceleration modes) have been collected as well as emissions during other than the FTP driving cycle in order to investigate the effect of average speed on vehicle emissions. These additional sources of data have been analyzed and appear, for the first time, in Supple-

Table 2. Past and ongoing emission factor programs.

Fiscal Year	Program	No. of Vehicles	Types of Vehicles	Test Sites	Test Procedures
1968	Rental vehicle surveillance program	705	1968-1969 automobiles	Los Angeles Detroit	7×7 FTP
1969	Great Plains surveillance program	2,029	1968-1969 light duty	Houston Kansas City	7×7 FTP
1970	National surveillance program, phase 1	2,101	0 light duty	Houston Kansas City Los Angeles Detroit Denver Washington	7×7 FTP
	National surveillance program, phase 2	369	1971 light duty	Houston Los Angeles Detroit Denver	7×7 FTP
	Surveillance study of smoke from heavy-duty diesel-powered vehicles, southwestern United States	64	1970-1971 heavy duty	San Antonio	Chassis dynamometer adaptation of 1970 FTP
	Surveillance study of emissions from heavy-duty gasoline-powered vehicles, southwestern United States	145	1970-1972	San Antonio	Chassis dynamometer version of 1970 FTP, over-the-road testing
1971	Study of emission from 1,020 light-duty vehicles in 6 cities	1,020	1957-1971 light duty	Chicago St. Louis Denver Washington Los Angeles Houston	1972-1975 CVS FTP, evaporative emissions, modal emissions
1972	Study of emissions from light-duty vehicles in 6 cities	1,020	1966-1972	Chicago St. Louis Denver Washington Los Angeles Houston	1972-1975 CVS FTP, evaporative emissions
1973	Acquisition of diesel truck operational parameters and emissions	10	1970-1973	San Antonio	Chassis dynamometer version of 1970 FTP, over-the-road testing
	Study of emissions from light-duty vehicles in 6 cities	1,080	1967-1974	Detroit St. Louis Denver Newark Los Angeles Houston	1972-1975 CVS FTP, modal emissions, evaporative emissions, loaded vehicle tests, air-conditioning tests, aldehydes and light HC, sound level tests, I/M correlation tests
	Mass emissions from precontrolled heavy-duty gasoline-powered vehicles	10	1965-1969	San Antonio	Chassis dynamometer version of 1970 FTP, over-the-road testing
	Ambient temperature and light-duty vehicle emissions	26	1967-1975 prototype	Bureau of Mines	1975 FTP
1974	Study of emissions from light-duty vehicles in 7 cities	1,968	1965-1975	Chicago Denver Houston Phoenix Washington St. Louis Los Angeles	1975 FTP, HWFET, modal, key mode, 2 short cycles, 2 other transient cycles, aldehydes and light HC
	Heavy-duty emission factor testing program (gas and diesel)	30	1965-1975	San Antonio	Steady state, sinusoidal, transient cycles, FTP
1975	Study of emissions from 6000-8500 pound GVW vehicles	250	1972-1976	To be determined	1975-FTP, HWFET, modal
	Study of emissions from motorcycles	200	1973-1976	To be determined	Proposed FTP, HWFET, modal
	Study of emissions from light-duty vehicles in 7 cities	2,220	1968-1976	Chicago St. Louis Phoenix Houston Denver Washington Los Angeles	1975 FTP, HWFET, modal, short cycles

ment 5 of Publication AP-42 (2). The methodology used to analyze these data will be discussed later in this paper.

The federal test procedures associated with heavy-duty vehicles are, at present, engine dynamometer exercises at warmed-up steady-state engine speed and load conditions. Unique procedures are applied to the gasoline-fueled and diesel engines and are known as the 9- and 13-mode test procedures respectively. The purpose of these test procedures was to measure emissions from heavy-duty trucks in all operational modes and not necessarily urban emission modes only. As a result, it was expected that changes in heavy-duty vehicle standards as measured on these test procedures might not reflect actual changes in urban on-the-road emissions. EPA surveillance programs have, therefore, tested with other test procedures in addition to the 9- and 13-mode tests.

The San Antonio Road Route (SARR) was selected by Southwest Research Institute as a characteristic urban road route for trucks. It tends to closely approximate the average speed and idle time in the light-duty FTP and has the advantage of measuring heavy-duty vehicles during actual operation in urban conditions. Acceleration-deceleration rates and speeds are not forced. EPA has sponsored surveillance testing of trucks on the SARR. In addition, during the past 2 years, EPA has collected a large base of heavy-duty truck operational data in preparation for the development of a representative urban transient driving cycle for heavy-duty trucks and buses. Preliminary subsets of these data have been used to develop different average speed transient cycles for trucks. These cycles have been incorporated into the most recent heavy-duty surveillance programs. Trucks have been tested at different average speeds and different loads in preparation for improvement of the emission factor data presented in Publication AP-42.

NEED FOR DEVELOPMENT OF EMISSION ADJUSTMENT FACTORS

The tabulated emission values in Publication AP-42 represent 1975 FTP emission performance levels for light-duty vehicles, light-duty trucks, and motorcycles. For heavy-duty vehicles, table values are SARR estimates for trucks operating in a warmed-up condition. Since CO is a localized pollutant, there are situations in which AP-42 table values need to be adjusted to more accurately simulate localized conditions. This adjustment is necessary because reductions in emissions from precontrolled base levels are not independent of operating mode.

Three examples are given. Table 3 gives the percentage of CO emission reduction from a base-line of precontrolled 1966 model-year vehicles as a function of model year-control system and hot-cold weighting. For reference, the 1975 FTP has a cold trip weighting factor of 43 percent as discussed earlier (percentage of trips beginning from a cold start). This should not be confused with the percentage of vehicle operating time or mileage in a cold condition.

Table 3 data indicate that, for pre-1975 production vehicles, the percentage reduction in CO emissions is essentially independent of hot-cold weighting although some indication exists that, for the 1968-1972 model-year vehicles, control was slightly greater during hot-start operation (cold transient weighting factor = 0.0) than during cold-start operation (cold transient weighting factor = 1.0). The table does not imply that absolute emission rates are independent of cold transient weighting factor.

Advanced emission control systems are not so stable with respect to hot-cold weighting. Catalyst systems, lean burn systems, and stratified charge systems provide greater reductions during hot-start operation than during cold-start operation. For example, certification data from 1975 catalyst vehicles indicate a 91 percent reduction from 1974 levels during hot-start operation and only a 77 percent reduction from 1974 levels for cold-start operation. Diesel and gas turbine engines provide slightly greater reductions during cold-start operation than during hot-start operation.

The percentage reduction in FTP composite CO emissions from precontrolled emission levels as well as the cold transient, hot transient, and stabilized bag emission reductions is given as a function of ambient temperature in Tables 4 and 5. Reductions achieved at 75 F (23.9 C) tend to be maximum reductions with the possible exception of the rotary engine. The differences between Table 3 and Tables 4 and 5 under standard FTP conditions are within the measurement uncertainty associated with the small sample sizes (25 vehicles) of Tables 4 and 5. Since the same vehicles were tested over the range of conditions in Tables 4 and 5, the trends rather than the absolute magnitudes are of major importance.

An indication of the effect of different average route speeds on CO emission reductions is given in Table 6; emission reductions increase as average speed increases. To reiterate, data in the table do not reflect absolute emission rates as a function of average speed but rather the percentage reduction in emissions from base-line levels measured over similar operating conditions.

Clearly, the use of adjustment factors will allow a much more accurate prediction of the present emission inventory at a localized site as well as the projected decrease in emissions resulting from the implementation of potential control strategies. Many localities have projected emission inventory decreases from 1970 to 1975 strictly by using the FTP emission factors without correcting for localized conditions. The potential overestimation of control can be seen by studying Tables 3, 4, 5, and 6. Cirillo, Norco, and Wolsko (3) support the concept that hot-cold weighted and speed-adjusted emission factors are better able to predict changes in ambient air quality than nonadjusted values.

CURRENT STATUS OF ADJUSTMENT FACTORS

Supplement 5 of Publication AP-42 (2) contains light-duty vehicle adjustment factors for hot-cold weighting, ambient temperature, and average route speed. A brief description of the basis for these factors is given. Although Publication AP-42 contains some adjustment factors for other than light-duty vehicles, these factors have been based on the light-duty vehicle data and associated analysis.

Hot-Cold Weighting Adjustment Factor

The adjustment factor can be defined as (desired hot-cold weighting)/(FTP hot-cold weighting). The equation can be expressed as

Adjustment factor = [(percentage of cold operation)(cold grams/mile)
+ (percentage of hot-start operation)(hot start grams/mile)
+ (percentage of stabilized operation)(stabilized grams/mile)]
÷ [20 percent(cold grams/mile)
+ 27 percent(hot start grams/mile)
+ 53 percent(stabilized grams/mile)]

$$\text{Adjustment factor} = \frac{wCT + xHT + (100 - x - w)S}{20CT + 27HT + 53S}$$

$$= \frac{w + x(HT/CT) + (100 - x - w)(S/CT)}{20 + 27(HT/CT) + 53(S/CT)}$$

Table 3. Percentage CO emission reduction as a function of hot-cold weighting factors.

Vehicle Description	Fiscal Year	Cold Transient Weighting Factor					
		0	0.2	0.43[a]	0.6	0.8	1.0
1966 models	1972	1.0	1.0	1.0	1.0	1.0	1.0
1967 models	1972	0.96	0.96	0.96	0.95	0.95	0.95
	1973	1.16	1.14	1.13	1.12	1.11	1.11
1968 models	1972	0.66	0.67	0.68	0.68	0.69	0.69
	1973	0.74	0.76	0.78	0.79	0.81	0.82
1969 models	1972	0.60	0.63	0.65	0.67	0.69	0.70
	1973	0.67	0.69	0.71	0.72	0.73	0.75
1970 models	1972	0.51	0.53	0.56	0.57	0.59	0.60
	1973	0.63	0.66	0.68	0.70	0.71	0.73
1971 models	1972	0.52	0.53	0.53	0.54	0.55	0.55
	1973	0.51	0.52	0.54	0.55	0.56	0.57
1972 models	1972	0.37	0.38	0.39	0.39	0.40	0.40
	1973	0.59	0.59	0.59	0.60	0.60	0.60
1973 models	1973	0.49	0.49	0.49	0.49	0.49	0.49
1974 models	1973	0.38	0.38	0.38	0.38	0.38	0.38
1975 models noncatalyst		0.085	0.098	0.096	0.099	0.103	0.107
1975 models catalyst		0.035	0.047	0.060	0.068	0.078	0.086
Production diesels		0.016	0.016	0.015	0.014	0.014	0.013
Multiple catalyst		0.017	0.021	0.026	0.029	0.032	0.035
Stratified charge		0.020	0.025	0.029	0.032	0.035	0.038
Lean burn		0.027	0.029	0.031	0.033	0.035	0.036
Turbine		0.046	0.044	0.041	0.040	0.038	0.036

Note: Emissions normalized to 1966 models tested in fiscal year 1972. Table is based on surveillance data, certification data, and EPA prototype vehicle test data.

[a] FTP.

Table 4. Percentage reduction in 1975 FTP CO emissions as a function of ambient temperature.

Vehicle	20 F	50 F	75 F	110 F
1967	1.0	1.0	1.0	1.0
1969-1970	0.53	0.43	0.39	0.39
1971-1972	0.57	0.46	0.36	0.45
1973-1974	0.54	–	0.36	0.51
Catalyst prototype	0.20	0.12	0.05	0.05
Rotary	0.12	–	0.16	0.20
Diesel	0.01	0.01	0.01	0.01
Proco (stratified charge)	0.01	0.005	0.005	0.005

Note: Normalized emission rates (1967 model-year vehicles used as base-line value). Data are based on 25 vehicles discussed in another report (4). (Deg F - 32)/1.8 = deg C.

Table 5. Percentage reduction in 1975 bag data CO emissions as a function of ambient temperature.

Vehicle	20 F			50 F			75 F			110 F		
	CT[a]	HT[b]	S[c]	CT	HT	S	CT	HT	S	CT	HT	S
1967	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
1969-1970	0.72	0.40	0.39	0.57	0.37	0.33	0.57	0.38	0.31	0.38	0.49	0.35
1971-1972	0.76	0.29	0.30	0.68	0.23	0.25	0.44	0.26	0.20	0.33	0.43	0.35
1973-1974	0.76	0.63	0.54	–	–	–	0.50	0.55	0.45	0.54	0.73	0.68
Catalyst prototype	0.43	0.06	0.01	0.29	0.05	0.01	0.10	0.06	0.01	0.08	0.10	0.01
Rotary	0.12	0.28	0.06	–	–	–	0.15	0.32	0.10	0.22	0.33	0.13
Diesel	0.01	0.02	0.02	0.006	0.02	0.01	0.009	0.01	0.01	0.01	0.01	0.00
Proco (stratified charge)	0.03	0.004	0.002	0.01	0.002	0.001	0.01	0.001	0.002	0.008	0.001	0.00

Note: Normalized emission rates (1967 model-year vehicles used as base-line value). Data based on data from 25 vehicles discussed in another report (4). (Deg F - 32)/1.8 = deg C.

[a] Cold transient bag emissions. [b] Hot transient bag emissions. [c] Stabilized bag emissions.

Table 6. Effect of average route speeds on CO emission reduction estimates.

Vehicle	5 mph	15 mph	25 mph	35 mph	45 mph
1957-1967	1.00	1.00	1.00	1.00	1.00
1968	1.13	1.07	0.93	0.84	0.77
1969	1.31	1.11	0.89	0.73	0.64
1970	1.52	1.12	0.89	0.71	0.61
1971	1.53	1.11	0.89	0.71	0.61

Note: Values are ratios of Publication AP-42 (5) speed adjustment factors for the year of interest to speed adjustment factors for the 1957-1967 base level. 1 mph = 1.6 km/h.

where

w = percentage of cold operation,
x = percentage of hot-start operation,
CT = cold grams/mile,
HT = hot-start grams/mile, and
S = stabilized grams/mile.

Surveillance and prototype vehicle data were examined to determine whether HT/CT and S/CT were dependent on vehicle model year or ambient temperature or both. The results indicated that model-year differences were not apparent before 1975, but catalyst vehicles were significantly different from noncatalyst vehicles. Temperature effects were similar for all noncatalyst vehicles but different from the catalyst temperature relations. For noncatalyst (pre-1975) vehicles, HT/CT and S/CT functions were identical. Linear regressions were performed on HT/CT and S/CT as a function of temperature (only 3 discrete temperature points were available) for the catalyst and noncatalyst cars. The results are given below for CO:

Car	Result
Noncatalyst HT/CT	$0.0045T + 0.02$
Catalyst HT/CT	$e^{(0.036T-4.14)}$
Catalyst S/CT	$e^{(0.035T-5.42)}$

The hot-cold weighting adjustment factor can be applied to Publication AP-42 table values as an independent factor only at 75 F (23.9 C). At other temperatures, the ambient temperature adjustment factor must be applied in conjunction with the hot-cold weighting factor so that the table values are adjusted to the FTP weighting at a given temperature before the weighting is changed. The hot-cold weighting factor has not yet been determined for other advanced emission control technologies.

Ambient Temperature Adjustment Factor

The ambient temperature adjustment factor can be defined as (FTP at T deg)/(FTP at 75 deg). Surveillance data and prototype catalyst vehicle data were examined to determine the temperature relation given above. Linear regression analysis indicated that pre-1975 vehicles had a different relation from prototype catalyst vehicles. The results are given below for CO:

Car	Result
Noncatalyst	$-0.0127T + 1.95$
Catalyst	$-0.0743T + 6.58$

No attempt was made to constrain the product of the hot-cold weighting factor and the temperature factor to a constant for the case of 100 percent stabilized operation. In addition, higher order regression was not attempted since correlation coefficients were above 0.9. The collection of additional data will allow these refinements to be evaluated; however, analysis of the present data base is limited by the existence of only 3 discrete temperature points. The ambient temperature adjustment factor has not been calculated for other advanced emission control technologies.

Average Route Speed Adjustment Factor

Using a large data base of modal emission data (5 steady-state modes and 32 acceleration-deceleration modes), EPA has developed a mathematical model that has the capability to calculate mass emissions of carbon monoxide (also hydrocarbons, nitrogen oxides, and fuel economy) emitted by vehicles during any specified driving sequence (4). This model provided the analytical tool for the development of speed adjustment factors. Urban driving data were processed to generate a large number of typical driving sequences with average speeds between 15 and 45 mph (24 and 72 km/h). These driving sequences were input into the mathematical model and predicted emissions were obtained. The predicted emissions were regressed against average speed by model-year vehicle and normalized to emissions at 19.6 mph (31.4 km/h). The CO relations for low altitude cities are given below where the general form of the adjustment factor is $e^{(A+BS+CS^2)}$.

Vehicle	A	B($\times 10^{-2}$)	C($\times 10^{-4}$)
1957-1967	0.967	-6.07	5.78
1968	1.047	-6.52	6.01
1969	1.259	-7.72	6.60
1970	1.267	-7.72	6.40
1971	1.241	-7.52	6.09

The current form of the regression model cannot be extrapolated below 15 mph (24 km/h) and can safely be extrapolated only to about 50 mph (80 km/h) on the high speed end. Supplement 5 (2) does provide discrete factors for idle, 5 mph (8 km/h), and 10 mph (16 km/h). A continuous model with speeds between 0 and 60 mph (97 km/h) is under development as is the inclusion of data for later model-year vehicles.

SENSITIVITY OF EMISSION PREDICTION

An understanding of the sensitivity of emission inventory calculations as a function of changes in various input parameters is of key importance for 2 reasons. First, such an analysis provides insight into which input parameters are most important to determine accurately. Second, such an analysis allows a policy maker to understand the uncertainty range and error implications associated with decision making. This section of the paper attempts to quantify the potential impacts of various parameters on the composite light-duty emission factor for calendar years 1980, 1985, and 1990. The following input parameters are considered:

1. Adjustment factors. The 3 adjustment factors described earlier are considered. Ranges for each factor are included along with interactive cases and the base case (case 1) represented by the 1975 FTP.
2. Growth rate. Growth rate has long been recognized as a problem input parameter. A base-case growth of 1 percent/year has been assumed for the purpose of estimating localized urban CO emissions. A low growth rate reflects the already congested urban situation.
3. Emission deterioration. The ability to predict future emission rates, long recognized as a model input problem, is dependent on a knowledge of emission standards and a knowledge of vehicle deterioration as a function of age and mileage. In this analysis, it is assumed that statutory CO emission standards will be introduced in 1978. However, deterioration rates are varied from the present estimates in Publication AP-42 (2) of 5 and 10 percent/year for noncatalyst and catalyst vehicles respectively to rates as high as 30 and 40 percent/year. This calculation has been included since the accurate definition of deterioration has been difficult and has been the subject of considerable EPA analysis.

Table 7 gives a description of the 15 cases examined in the sensitivity study. An attempt was made to include a variety of localized scenarios as well as growth rate and deterioration rate changes. Table 8 gives a summary of the results. Although growth rate and deterioration (future emission factors) have long been recognized as critical to model prediction, data in Table 7 indicate that both absolute emission readings and percentage reduction of emissions over the projection period are highly dependent on the specific set of adjustment factors used. The presence of low ambient temperature with cold vehicle operation results in maximum emission and emission reduction differences from base-case conditions. Thus, the use of adjustment factors is as critical to accurate projections as are factors such as growth rate and emissions from future emission control technologies.

FUTURE WORK AREAS

Analyses such as those presented in this paper indicate the need to continue to refine the emission factor estimates in Publication AP-42. Refinement includes updating projections of FTP emissions as a function of vehicle age for each mobile source category as well as developing adjustment factors. This section highlights those areas that are currently undergoing refinement and those areas that are planned for the near future.

Table 7. Description of cases for sensitivity study.

Case No.	Case Description	Temperature (F)	Hot-Cold Weighting CT[a]	Hot-Cold Weighting HT[b]	Hot-Cold Weighting S[c]	Speed (mph)	Growth Rate (percent/year)	Deterioration (percent/year) Catalyst	Deterioration (percent/year) Noncatalyst
1	Urban average	75	20	27	53	20	1	10	5
2	Morning rush hour	80	0	0	100	20	1	10	5
3	Afternoon rush hour	80	100	0	0	20	1	10	5
4	Urban average	20	20	0	80	20	1	10	5
5	Urban average	40	20	0	80	20	1	10	5
6	Intersection	80	20	0	80	5	1	10	5
7	Highway link	60	0	0	100	45	1	10	5
8	Parking lot	20	100	0	0	5	1	10	5
9	Intersection	20	20	0	80	5	1	10	5
10	Urban average	75	20	27	53	20	1	20	10
11	Urban average	75	20	27	53	20	1	30	20
12	Urban average	75	20	27	53	20	1	40	20
13	Urban average	75	20	27	53	20	0	10	5
14	Urban average	75	20	27	53	20	2	10	5
15	Urban average	75	20	27	53	20	4	10	5

Note: (Deg F − 32) ÷ 1.8 = deg C. 1 mph = 1.6 km/h.

[a] Cold transient [b] Hot transient [c] Stabilized

Table 8. Light-duty vehicle CO emission rate and percentage reduction sensitivity to input parameters.

Case Number	1972 Emission Rate[a] (g/mile)	1972 Reduction (percent)	1980 Emission Rate[a] (g/mile)	1980 Reduction[b] (percent)	1985 Emission Rate[a] (g/mile)	1985 Reduction[b] (percent)	1990 Emission Rate[a] (g/mile)	1990 Reduction[b] (percent)
1	69.3	0	24.5	65	8.78	87	4.68	93
2	47.8	0	14.0	71	3.19	93	0.79	98
3	125.7	0	56.3	55	16.5	87	9.12	93
4	115.1	0	59.0	49	32.1	72	22.8	80
5	97.8	0	45.7	53	23.0	76	15.7	86
6	204.8	0	80.8	61	24.8	88	10.3	95
7	24.0	0	6.0	75	1.31	95	0.32	99
8	1291.0	0	989.5	23	620.4	52	462.2	64
9	371.9	0	240.8	35	135.8	63	96.4	74
10	69.3	0	30.5	56	11.5	83	6.12	91
11	69.3	0	40.9	41	15.3	78	7.44	89
12	69.3	0	42.2	39	17.1	75	8.76	87
13	69.3	0	22.7	67	7.70	89	3.90	94
14	69.3	0	26.6	62	9.93	86	5.58	92
15	69.3	0	31.1	55	12.9	81	7.92	89

Note: Data based on application of Supplement 5 (5) emission factors and adjustment factors. 1 g/m = 0.6 g/km.

[a] Adjusted to include growth so that base mileage can be considered constant [b] Computed from 1972 base year case

Light-Duty Vehicle Speed Adjustment Factors

Work is ongoing to develop a continuous adjustment factor to span the range from idle to 60 mph (96 km/h) as a function of the model-year and emission control system. The adjustment factors for precontrolled through 1975 model-year vehicles are projected to be completed by July 1976. Publication AP-42 currently assumes post-1971 model-year vehicles have the same speed adjustment factors as 1971 models.

Light-Duty Vehicle Temperature and Hot-Cold Weighting Adjustment Factors

Work is scheduled to begin in fiscal year 1976 to expand the data in Publication AP-42, Supplement 5. Temperature ranges will be expanded to include 0 to 100 F (17.8 to 37.8 C) as well as advanced emission control technology vehicles. Continuous emission trace analysis will be employed to more accurately define the time after vehicle start-up at which emissions stabilize, the effect of soak time on vehicle start-up emissions, the effect of vehicle soak time on vehicle emission stabilization, and the effect of different driving cycles on emission stabilization time. Completion of this project is estimated to be December 1976; there may be intermediate outputs. Final results are projected to include soak time correction factors.

Interaction of Light-Duty Vehicle Adjustment Factors

Data are currently being collected on 1968-1975 model-year vehicles to verify that the existing adjustment factors are independent. For example, the assumption that emissions from vehicles operating during a 5-mph (8-km/h) cold driving sequence can be calculated by multiplying a 5-mph speed factor by a 100 percent cold factor will be checked. Corrections will be developed as needed. This work is scheduled for completion July 1976.

Light-Duty Vehicle Road Grade Adjustment Factor

In adjustments for highway ramp situations, road grade is often of importance. A small work effort will be undertaken in fiscal year 1976 or 1977 to investigate this effect. An adjustment factor is projected by December 1976.

Light-Duty Vehicle Load Adjustment Factor

Data have been collected on a sample of pre-1975 model-year vehicles at 3 load conditions. These data will be developed into an adjustment factor by July 1976.

Light-Duty Vehicle Emission Update

Data are currently being collected in 7 U.S. cities on 1968-1975 model-year vehicles to update the FTP emission rates in Publication AP-42. Analysis work will continue to update deterioration estimates as well as examine whether deterioration with age and mileage varies as a function of driving sequence. A follow-on test program is scheduled to begin in January 1976 to continue testing 1970-1975 vehicles as well as 1976 model-year vehicles. Diesel light-duty vehicles will also be tested.

Light-Duty Truck Emission Update

Data will be collected on 1972-1976 model-year [6,000 to 8,500 lb (2722 to 3856 kg)

GVW] light-duty trucks. These data will allow light truck emissions to be updated as a function of age and mileage. In addition, speed adjustment factors will be calculated for trucks as heavy as 8,500 lb (3856 kg) GVW. Publication AP-42 currently assumes that light-duty vehicle speed adjustment factors are appropriate. This data base will also be used to check the applicability of light-duty vehicle hot-cold weighting adjustment factors to trucks as heavy as 8,500 lb (3856 kg) GVW. Completion date is estimated to be December 1976.

Motorcycle Emission Update

Data will be collected on 1973-1976 model-year motorcycles. These data will allow motorcycle emissions to be updated as a function of age and mileage. In addition, speed adjustment factors and hot-cold weighting adjustment factors will be calculated. Publication AP-42 currently assumes light-duty vehicle adjustment factors are appropriate. Completion date is estimated to be December 1976.

Heavy-Duty Vehicle Speed Adjustment Factors

Data are being collected on both heavy-duty gasoline and diesel trucks for a variety of different speed driving sequences. These data will be developed into equational speed adjustment factors by fuel type and emission control system. Work should be completed by July 1976. Publication AP-42 currently assumes light-duty gasoline speed adjustment factors apply to heavy gasoline trucks. It now provides diesel speed adjustment factors by using a modal interpretation of the 13-mode engine test.

Heavy-Duty Vehicle Load Adjustment Factors

Data are being collected on both gasoline and diesel trucks for 3 load conditions at many different average speeds. These data will be developed into equational load adjustment factors (probably as a function of speed) by fuel type and emission control system. Work should be completed by July 1976.

Heavy-Duty Emission Update

The data base referenced above will approximately double the surveillance data on heavy-duty vehicles. These data will be used to update the basic heavy-duty emission factors in Publication AP-42. Work is projected to be completed by July 1976.

Light-Duty Vehicle Inspection and Maintenance Update

Inspection and maintenance were not included in the sensitivity study since present in-house data analyses indicate that the maximum potential effectiveness of inspection and maintenance depends on the specific implemented program and the capability of the service industry rather than the model-year vehicle-emission control system-localized operational situation. A large-scale pilot program is planned for fiscal years 1976-1977 to assess the effectiveness of inspection and maintenance as a function of each of the parameters discussed above. Analysis will not be complete for some time. An assessment of the mandatory, but nonenforced, Chicago inspection and maintenance program is planned for January 1976.

Development of a Computerized Version of Publication AP-42 Mobile Source Emission Factors

As the complexity of the mobile source emission factors increases, the job of calculating a composite mobile source emission factor for a given calendar year is difficult even after the accumulation of input data is completed. At the present time, such calculations are time consuming to complete by hand or with small desk calculators. Future refinements to the emission factors will increase the problem. EPA is developing a computerized version of Publication AP-42 that attempts to be general. The user will be able to input any specified set of operational conditions. Growth rates, mobile source category mix, and distribution of vehicles by age can be changed easily in the input data files. EPA intends to keep this program current with the available supplements and to provide it to interested users. Users would have the option of using national or selected regional inputs or both on growth and vehicle distribution or of modifying input files. Work on this project is under way, but it is not projected to be completed until July 1976. At that time, a reference document along with instructions for obtaining the program will be made available.

CONCLUSIONS

Available air quality models provide a tool for projecting future ambient air quality levels from a knowledge of present ambient air quality levels and present source emission levels. Because of the localized nature of carbon monoxide problems, it is extremely important to isolate the conditions that result in hot spots in order that future projections will indeed predict worst case situations. The analyses presented in this paper strongly support the fact that carbon monoxide projections based on average urban conditions may grossly underestimate or grossly overestimate absolute emission levels or percentage changes in emission levels from a base year of interest.

EPA has expanded and is planning continued expansion of mobile source adjustment factors. These adjustment factors provide a method to obtain localized emission factors from federal test procedure or average urban emission factors (federal test procedure emission factors tend to better estimate areawide pollutant impact). In addition, EPA will continue to improve its average urban emission factors as a function of vehicle age and mileage for each mobile source category and major emission control technology within each category. Although there is no set time for publication of mobile source updates, they will be published when major new data become available, approximately once per year. The projected publication date of the next supplement is July 1976.

The increasing complexity of mobile source emission factors places 2 burdens on the users of these data. First, the data are difficult and time consuming to manipulate computationally. EPA hopes to alleviate this problem by computerizing the mobile source portions of Publication AP-42 and providing this capability to users. Second, the available input data needed to take full advantage of the adjustment factors are not always readily available.

Whenever possible, localized data on growth rates, vehicle mix, and vehicle age distribution should be obtained from traffic surveys. Data on ambient temperature can be obtained easily from airport monitors, and localized effects on any given day can be expected to be small. Data on average speed are also reasonably easy to obtain. Such data can be obtained by timing probe vehicles as they traverse the localized area of interest. Hot-cold weighting estimates (and load factor estimates when they are included) are the most difficult inputs to obtain. In cases where they cannot be obtained, it is recommended that a range of values be examined with a worst case estimate included.

SUMMARY

Ambient air quality modeling of carbon monoxide is dependent on accurate mobile source emission factors. The paper examines the sensitivity of emission factor projections to input parameters such as ambient temperature, hot-cold weighting, average route speed, vehicle deterioration, and growth rate. The ability to estimate cold vehicle operation at low ambient temperature is as important to localized emission prediction as is the estimation of growth rates and emissions from future emission control technology vehicles. Analysis of existing data indicates that localized emission factors are needed since projected reductions in emissions from base-line levels are not independent of vehicle operating mode. Present emission factors and planned refinements to EPA Publication AP-42 are discussed.

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AMBIENT AIR MONITORING FOR HIGHWAY ENVIRONMENTAL ANALYSIS

F. L. Palmieri, Air Quality Analysis Unit, New York State Department of Transportation

The ever-increasing demands for accurate analysis of air quality impacts of highway proposals have caused ambient air quality monitoring to become a topic of substantial concern to transportation analysts. The data acquired through ambient air monitoring are an essential input to the mathematical models used for highway air pollution forecasting, both for the determination of ambient background levels and for the validation and calibration of the models themselves. Despite its importance, however, a standardized body of procedure and good practice for this type of data acquisition has developed slowly. Because of the substantial differences between this type of ambient monitoring and that done routinely by state environmental agencies for their urban-area air quality surveillance programs, the techniques for highway ambient monitoring have largely grown out of the efforts and experimentation of the state and federal transportation agencies themselves. This paper presents some of the considerations and results of such an effort by the New York State Department of Transportation, which has had an active and extensive program in this field since 1972.

USES OF AMBIENT AIR DATA

Because the uses to which the data will be put have a great influence on the data collection process, the 2 primary purposes of the ambient monitoring effort should be briefly reviewed.

First, and most straightforward, is the acquisition of ambient data for the purpose of estimation of background concentration. Most of the standard mathematical models in use for highway analysis provide forecasts only of the pollution contribution from the highway; to this must be added an estimate of future contributions from other sources. A standard procedure for doing this is first to measure present-day background levels in the vicinity of the proposed project site and then to adjust these measurements to provide future forecasts by some sort of "rollback" analysis making use of the estimates of future areawide emission levels to be found in the state air quality implementation plan.

A more subtle and complicated use for ambient data is in the validation and calibration of the predictive models themselves. Most highway departments currently involved in this kind of analysis make use of Gaussian-diffusion models, such as the FHWA and California Division of Highways TLINE and CALINE or the U.S. Environmental Protection Agency HIWAY. The direct usefulness of these models is limited. They are derived for a certain set of specific and limiting assumptions, including constant vertical wind-speed distribution, constant wind direction, uniform wind flow field upwind of the highway section, no obstructions off the highway or sharply sloped cuts or fills adjacent to it, no aerodynamic effects of flow about supporting structures, and so forth. As a result, predictions made by use of these models are only applicable—without further calibration—to the case of a rural, at-grade highway. For any more complex situation, including the important urban situations of cut sections, elevated sections, and street canyons, a calibration of the model should be done. This allows correction of the model for violations of the input assumptions, which would otherwise be unaccounted for and could introduce serious errors.

Lately there has been increasing use of the new generation of numerical or conservation-of-mass models. These, even more than the Gaussian models, require extensive programs of ambient data acquisition to successfully validate and calibrate them.

It must be kept in mind that, when we speak of calibration of a model, we are perforce talking about a more complex monitoring effort than would be required simply for the determination of ambient background concentrations. To provide a valid calibration requires that concentration measurements be obtained at 2 points at least on each side of the roadway at a given cross section of interest. The calibration analysis then becomes an effort to determine the single calibration constant that gives the best "averaged" predictive curve matching the 4 (or more) measured points. Obviously a true calibration cannot be made with only a single measurement point since the calibration constant would only ensure a match between the model and observed reality at this 1 point, with no assurance of acceptable predictive accuracy anywhere else.

APPROACHES TO DATA ACQUISITION

There are obviously several approaches by which the necessary data may be gathered. If the primary object is to determine ambient background concentration data, using some existing source of this information may suffice. The most common source is the ambient data taken in each urban area as a part of each state's ambient air quality surveillance system. Although originally intended for the purpose of measuring progress toward achievement of the National Ambient Air Quality Standards and providing the data input necessary for an air quality emergency episode warning system, these urban networks (sometimes referred to as continuous air monitoring systems or CAMS) can provide useful data to the transportation planner. The most serious weakness of CAMS as sources of ambient data is that generally the funding available for the network limits it to a small number of monitoring stations, and these are generally located to observe the most serious concentrations of stationary pollution sources in the area. These locations may or may not be at all suitable with respect to providing meaningful data for the transportation corridor under study. Nevertheless, CAMS should certainly be among the first data sources considered by the transportation planner not having his or her own monitoring capability.

Similarly, it may be found that there exist other sources of ambient data that were gathered for other special purposes. For example, under state indirect source control regulations, developers of major commercial enterprises may be required to do ambient monitoring in support of the air quality impact analysis that must accompany the indirect source permit application. Or, a local university may conduct air quality monitoring for academic or research purposes. A good starting point for attempting to identify significant sources of existing ambient data is the U.S. Environmental Protection Agency data bank (storage and retrieval of aerometric data, or SAROAD). SAROAD receives data from a variety of sources, codes them by geographic location, and tabulates them in a standard format for easy retrieval. It can often provide clues to the existence of ambient data that would otherwise go unnoticed.

Should secondary sources such as CAMS and SAROAD fail to provide suitable data, the transportation agency faces the necessity of performing a special monitoring study. This may often arise when ambient background estimates are prepared, and is virtually inevitable when one is involved in the calibration of mathematical models. Again, the agency has several possible approaches: It may have the data gathered for it by some outside group under contract, by another governmental agency, or by a private consultant; or it may choose to establish its own monitoring program. Many transportation agencies whose monitoring needs are limited will choose the consultant-contract option. This approach, however, has distinct advantages and disadvantages that should be clearly understood in advance.

The basic administrative advantage of using a private consultant is, of course, the saving in time and administrative effort compared to that required for the agency to establish its own monitoring program. Especially now, when widespread fiscal crises and consequent austerity programs affect many state governments, the establishment of an in-house monitoring program, with its attendant problems of civil service staffing procedures and equipment purchase justifications, may simply be unfeasible from an administrative point of view. In such a case, consultants who can provide their own equipment and technicians and who furnish as a final product ready-to-use, edited tabulations of the necessary data, will seem attractive. This is especially true if the data are needed quickly; even in the best of times, the cumbersome budgetary procedures of most state governments would require at least 1 to 2 years of lead time to establish an in-house program.

On the other hand, the use of consultants may be a foolish choice to the agency whose program will clearly require a large-scale, continuing monitoring effort in support of a steady stream of environmental impact statements (EIS). The costs involved in consultant production of data have, in our experience, ranged from 2 to 4 times the unit cost of producing the same data via an in-house program. Such costs can quickly become unbearable if the overall scale of the program is large.

The transportation agency facing the need for a monitoring program of such magnitude may choose to contract for the data acquisition by another government agency, rather than try to establish its own program. Because of the air-surveillance requirements of the Clean Air Act Amendments of 1970, each state and many regional or local environmental agencies are now deeply involved in ambient data collection. Administratively, it is quite possible for the least cost and least effort solution to the transportation monitoring requirement to be the establishment of a special monitoring program, catering to the highway EIS requirement, within the environmental agency's overall monitoring effort. There are many obvious advantages of such an approach, including centralized management responsibility, use of established personnel pools, avoidance of the need for separate and duplicative maintenance and repair facilities and spares inventories, and acquisition and editing of the data to uniform, national EPA standards of quality assurance by personnel experienced in proper procedures.

In fact, this was the approach adopted by the New York State Department of Transportation (NYSDOT), which in early 1973 established such a joint program with the New York State Department of Environmental Conservation (NYSDEC). Initially, NYSDOT provided full funding for the acquisition of 5 fully equipped mobile laboratories and ancillary equipment (totaling about $250,000), and NYSDEC provided personnel, expendable supplies, and computer facilities for data tabulation. In subsequent years, NYSDOT has furnished lower levels of funding sufficient to cover equipment and material expenses and a proportion of the personnel costs. The joint program has been highly successful overall, producing good data at a much lower cost than had been estimated for a fully in-house NYSDOT program.

It may, of course, be that an individual transportation agency finds that such an option is not open to it. The appropriate environmental agency may find its resources already committed to such an extent that it has no interest in assuming additional responsibilities, even if partly or wholly funded by the transportation agency. Or, in some states, the environmental agency may have delegated the monitoring responsibility to local agencies who prove uncooperative for a variety of reasons. In such a circumstance, the transportation agency will have little choice (if the scope of its program precludes use of private consultants) but to establish its own in-house monitoring effort. The remainder of this paper will be devoted to a discussion of some of the considerations central to the establishment of such a program, on either a joint or fully in-house basis.

PERSONNEL FOR THE MONITORING PROGRAM

One of the more difficult problems that must be faced is the acquisition of appropriately skilled personnel. Ambient air monitoring is a highly specialized branch of physical chemistry, demanding personnel possessing training and skills not usually available in the typical transportation department. These personnel will fall into 4 general categories: monitoring program managers, instrumentation operators, maintenance and repair technicians, and data editing, processing, and tabulation specialists.

The monitoring program manager must be a highly skilled jack-of-all-trades. He or she must have extensive background in the theory and practice of monitoring instrument operation while also having a familiarity with basic transportation planning procedures and with the requirements of the mathematical modeling of pollutant dispersion that will affect technical decisions on the monitoring (e.g., site selection and location of probes). Personality and ability to work well with associates of widely varying backgrounds will be of great importance since he or she will be a personal bridge between the transportation planners, usually highway planners and designers, and personnel whose whole training and orientation are toward environmental studies, which in some cases will have developed in them a definite antagonism toward the whole highway program. Under such circumstances, considerable diplomatic abilities are a necessity.

The equipment and mobile laboratory operators will generally be junior scientists, generally having an environmental-studies background and a fairly recent bachelor's degree. They must be capable of operating all the equipment and evaluating the validity of data on a real-time basis to detect malfunctions as early as possible and be trained to perform basic service and repair work. One of the more difficult problems associated with the use of such personnel is the difficulty in retaining them in a job that is an endless round of physical moves, with little time at any permanent home. For this reason, experience indicates that the young unmarried person best fills this sort of position; however, one may have to be resigned to, and prepare to deal with via vigorous recruitment, a rather higher job-turnover rate than is customary in government agencies. An advantage of the cooperative-program approach discussed above is that within the environmental agency will probably be a number of advancement opportunities open to the laboratory operator, thus tending to ameliorate his or her growing unrest with the unsettled nature of the job. Opportunities for career advancement for a person of such a background are generally much rarer in a transportation agency; therefore, the employee may come to think of the job as merely a waystop on the way to better things elsewhere. Obviously such an attitude is not conducive to high productivity.

The electronics technician may pose far fewer problems for the transportation agency. Generally some personnel of such a background will already have been retained for use in servicing traffic-count and other programs already making use of sophisticated electronic equipment. Therefore, the agency may find it easiest to build on its existing management and workshop capability, adding a small number of suitably trained workers as necessary. Specialized training in the maintenance of monitoring instruments is often available from the manufacturers; the EPA Institute for Air Pollution Training also offers introductory-level courses in instrumentation that can be highly useful in the basic indoctrination of skilled personnel.

Similarly, most transportation planning agencies will already have substantial in-house capability for data processing and tabulation by computer. Again, the EPA institute courses provide a useful introduction to the specifics of air quality data handling.

SELECTION OF EQUIPMENT

Equipment selection is the next crucial problem facing the monitoring program manager. If he or she is to be successful in equipping the unit to carry out its responsibilities within the typically insufficient budget, careful attention must be paid to some preliminary considerations.

First is the question of selecting the pollutants to be monitored. Obviously, carbon monoxide is the first and most important choice. Generally, whenever any monitoring at all is required in connection with a transportation EIS, carbon monoxide will be the most important—and often only—concern. Beyond CO, however, the monitoring program manager should proceed cautiously.

Certainly nitrogen oxides and nonmethane hydrocarbons are transportation-related pollutants that must be discussed in the air quality analysis of any major transportation project. However, monitoring for these pollutants is not automatically justified. At the present, there are no widely accepted photochemical models for the dispersion of these pollutants. Therefore, they are normally treated in an EIS on a mesoscale basis; that is, any concentration calculations are normally based on simplistic box or rollback models. It may, therefore, be argued with considerable logic that the acquisition of extensive NO_x and HC data, specific to the proposed highway location, is not justified. The alternative would be to make use of CAMS or other existing data, arguing that it will provide an area-average estimate of existing concentrations that is conceptually consistent with the crude, areawide model used for these pollutants. I feel that, if such data are available from other sources and do seem to be usable within such a philosophical framework, the transportation agency may be much better off to put its money into acquiring additional CO monitoring instruments, thus allowing the measurement of CO at several points in space at a given cross section and allowing better model calibration.

Another question requiring an early answer relates to the necessary extent of meteorological monitoring. If the agency is confining itself to the use of the simplest Gaussian-diffusion models, applied in cross-sectional geometries consistent with their assumptions, and dealing with an environmental review agency that will accept the use of an uncalibrated model, little meteorological monitoring may be required. The agency may be able to confine its acquisition of meteorological equipment to a small number of self-contained wind speed-direction units, such as the well-known MRI mechanical weather station. At the other extreme, in a major project in a heavily polluted urban area and in the presence of complex geometries of cross sections and obstructions, a sophisticated, calibrated model is a necessity. Under such circumstances the meteorological equipment inventory will be larger both in number of instruments (due to the need to monitor more points in space at a given cross section) and in sophistication (due to the need for esoteric data such as 3-axis wind components and vertical and horizontal stability parameters).

In the latter case careful attention will have to be paid to specific choice of equipment since many of the most useful instruments on the market, in terms of their sensitivity and range of output parameters, are designed primarily as research tools and do not possess the durability required for long-term monitoring at exposed sites under all weather conditions.

Having arrived at the requisite decisions regarding the scope of his or her program, the monitoring program manager must next proceed to choose field instrumentation. In this, there is really no substitute for long experience; some equipment may exceed every specification and expectation, while other equipment may exhibit only the most tenuous relation between catalog claims and actual field performance. If the program manager has limited experience in the field, he or she ought to seek available expert opinions from environmental agencies, local academic institutions, or any other handy source. For further guidance, a few general principles might be stated at this point.

The longevity in business and the service record of the manufacturer should be considered. The air monitoring equipment field, especially in the last few years, has seen numerous small manufacturers come into existence, place equipment in service, and then disappear into mergers and bankruptcies, leaving customers with expensive inventories of "orphan" instruments for which parts and service are no longer available.

Cost, therefore, should not be allowed to be the paramount consideration since most often the marginal producer will be able to quote a somewhat lower price than the large manufacturer whose quoted price must include a fair share of corporate overhead costs. This is certainly not to say that one should avoid the small manufacturer and deal only with the giants of the industry. But the purchaser should clearly understand the possibilities of the situation. Of course, the small manufacturer may quote a price on the basic instrument and an adequate inventory of spares that in total is still lower than the larger company's instrument price alone. Then, as long as the purchaser is confident of his or her in-house service capability, there is no reason not to take advantage of the cost break.

Those agencies whose monitoring unit personnel will be thinly stretched will want to carefully investigate the newer generation of instruments that provide a self-calibration capability. In combination with a data telemetry system and some automatic checks for validity as the data are fed into the computerized tabulation system so as to quickly identify equipment failures, these self-calibrating instruments may greatly reduce or eliminate the need to have an operator physically present. Instead, the mobile laboratory or instrument installation may simply be set up in a secure place, protected from vandals, and merely visited periodically by a technician performing routine preventive maintenance. Or, if necessary, an operator may be able to divide his or her time between several installations in the same general area.

SPECIFIC TYPES OF INSTRUMENTATION

Although it is not appropriate here to discourse at length on the various types of instrumentation available, agencies only now beginning to build a monitoring capability may perhaps benefit from a brief discussion of the experiences of the New York Department of Transportation with the various specific units now in use for the production of data to support highway EIS preparation.

For carbon monoxide, we at first made the same choice as a number of other agencies and acquired a substantial number of electrochemical CO analyzers, primarily for their great cost advantage over other types of CO monitors. However, it must be candidly stated that in the long-term continuous monitoring application these units did not work out well and have been superseded by other instruments. The basic problem was simply that they were not originally designed or intended for long-term continuous operation and, therefore, constantly had difficulties of component durability and calibration drift. Used for their designed purpose—short-term, spot monitoring, with frequent calibration and no extended on-cycles—they can be quite useful. But in the continuous monitoring application, they were not equal to the demands placed on them. Many agencies have purchased these units or are currently considering their purchase, primarily because of their potentially tremendous cost savings (they are about one-third the cost of an infrared spectrometer), but I feel strongly that their acquisition should be accompanied by a clear understanding of their strengths and weaknesses. Also, in fairness to the manufacturer, I should point out that since our purchase considerable development work has taken place on the instrument and late models may exhibit substantially improved durability.

In our mobile laboratories, until recently the primary instrument for both carbon monoxide and hydrocarbons was the gas chromatograph/flame ionization detector (GC/FID). These units performed well, but at the cost of high personnel demands for servicing and calibration. The other inherent disadvantages of the GC/FID, including the need for highly flammable hydrogen fuel and extremely high cost, are well-known and need not be belabored here. Nevertheless, they were significant enough that, when a decision was made to discontinue acquisition of HC data as a routine practice, we decided to replace them with infrared photometers for CO.

The nondispersive infrared photometer (NDIR) is, of course, the classic method of CO determination and is the original EPA-approved reference method for this pollutant. We originally shied away from NDIR equipment largely because of the bad experiences of other agencies with interferences and calibration drift when this type of instrument was used for long-term, unattended operation. However, an evaluation of the latest generation of self-calibrating NDIRs convinced us that these problems appear to have been reduced to manageable proportions in a properly installed instrument, and we now use these exclusively for CO measurement. We have not had them on hand long enough to say anything definitive about long-term durability, but the results of the evaluation tests performed for us by the service personnel of the Department of Environmental Conservation certainly seem promising.

The comments above on the gas chromatograph for CO determination apply equally well to its use for hydrocarbons. It is the only practical instrumental method currently available. Although it produces good data, the operational difficulties associated with using it in a mobile field application are serious enough to warrant second thoughts about whether the HC data acquisition is really necessary and justified.

The original EPA-approved reference method for nitrogen oxides is the modified Saltzmann method, a wet-chemistry technique. Although perhaps suited to laboratory use, I know no one actively engaged in a transportation monitoring program from mobile laboratories who seriously considers it a practical method. Further, of course, the accuracy of the method has been under serious challenge, and EPA has withdrawn it as a reference method. EPA has subsequently proposed alternative wet-chemistry methods that eliminate the accuracy problem, but all have the basic impracticality of dealing with glassware and reagents in a field operation, compared with the use of an electronic instrument. Therefore, the use of instruments operating on the chemiluminescent principle is almost universal for highway monitoring. These have performed well for us, given proper installation and service. Particular attention must be paid to proper control of the ethylene, which these instruments use as a working fluid. A leak in the exhaust plumbing or placement of the exhaust outlet too close to the intakes for other instruments, can create serious interferences, especially with the gas chromatograph, which determines nonmethane hydrocarbons by first making a total hydrocarbon measurement, which would include the spurious ethylene as well as ambient hydrocarbons.

We originally equipped our mobile laboratories for determining ozone but the data have proved to be of only limited usefulness, and we have effectively discontinued regular O_x monitoring. Similarly, our HiVol particulate samplers have seen only limited use because of the limited emphasis placed on particulates from transportation sources by our environmental review agencies.

HOUSING THE EQUIPMENT

There are 3 common approaches to housing the equipment: use of existing local buildings, use of special small shelters, and use of mobile laboratories. Each has some particular advantages and disadvantages for the monitoring program manager to consider before selecting the approach.

The use of local buildings may be attractive when suitable structures are available in appropriate locations. The obvious advantages will be low (or no) cost and, usually, ready availability of utilities. On the other hand, security from vandalism may be a problem. Tenants of the building may object to noise from the instruments. The explosive gases required for GC or chemiluminescent equipment may constitute a violation of local fire regulations. Owners of private buildings may insist on payment for electricity and other utilities (if drawn from existing building circuits) and on prearrangement for liability indemnification in the event of an accident. Most important, a suitable building simply may not be available at the desired monitoring site. Nevertheless, despite these potential problems, the program manager is always well-advised to look for a building location first.

If a suitable building is not available, use may be made of some sort of small, easily erected and removed shelter—usually a small metal hut just big enough to comfortably enclose the equipment. If the study is to be of extended duration and the equipment is self-calibrating and does not require constant attendance, this may be the most cost-effective solution. However, it may be a poor choice (in the absence of a security system) at high-security-risk locations since such a structure is usually rather flimsy and presents little challenge to the vandal determined to break in. Also, the precise control of environmental factors such as temperature and humidity, which are crucial to the proper operation of some instruments, may be difficult to achieve in such an unsophisticated structure. Despite these problems, its very low cost makes the small shelter an attractive alternative, especially to the agency whose overall monitoring program is of limited or uncertain scope.

The mobile laboratory is an approach that has been adopted in a number of states. The laboratory offers good opportunity for environmental control; adequate interior space for multiple instrumentation as used in a sophisticated calibration study; provision for an on-the-spot maintenance and repair capability; and great flexibility in location. It also permits the use of instruments that require the constant presence of an operator; or, alternatively, the headquarters space may be used for real-time monitoring of the data, or even for a security guard. In the latter context, also, the laboratory (especially if it is a towed trailer) can be much more sturdily built than the small shelter. If security is a consideration from the beginning of its design, it can be made reasonably invulnerable to casual vandalism.

The laboratory may provide surprising protection to its valuable cargo of instruments in an accident situation. We discovered this when one of our laboratory trailers came adrift from its tow hitch at 55 mph (88 km/h) on the New York State Thruway. The trailer left the road and was thoroughly demolished, but the solidly mounted equipment suffered only relatively minor damage and was soon repaired.

A major decision in considering the mobile laboratory approach centers around the question of whether the unit should be self-propelled and self-powered or towed and dependent on external utility hookups. There are trade-offs involved in all aspects of this decision. The self-propelled laboratory will be much more mobile; but, if it is to move only once every few months, is the mobility worth the cost? On the other hand, in security-risk areas, the mobility may pay for itself many times over if vandalism is avoided by withdrawing the unit to a safer location each night. The self-powered laboratory is far more flexible in terms of where it can be installed, but it may be far more expensive to operate, and the generator exhaust may affect the instrumentation.

Balancing all these considerations, we chose an externally powered, towed configuration; however, varying conditions of use could equally validly lead monitoring program managers in other states to different choices. The most important part of the decision-making process will always be a careful evaluation of the operational conditions under which a laboratory will be used, with no preconceptions as to the type or configuration of vehicle. The application should generate the specifications.

CONCLUSION

This paper can only introduce an exceedingly complex topic. It presents an array of information and advice to those who are new to ambient monitoring. For that reason, it is appropriate to close by repeating a statement made several times previously: Monitoring is definitely a field in which experience is the best teacher. The wise monitoring program manager, especially a neophyte, will keep open all possible lines of communication with agencies and individuals already working in the field. This includes EPA, state and local environmental agencies, appropriate academic groups, and other state transportation agencies.

MICROSCALE CARBON MONOXIDE CONCENTRATIONS AND WIND CHARACTERISTICS ON NEW YORK CITY STREETS

Gary L. Latshaw, Wolfgang Schaechter, Marilyn H. Taynai, and Benjamin B. Hulet, Environmental Systems Laboratory Inc., Sunnyvale, California; and
John F. Sontowski and Lewis E. Guthman, New York City Department of Air Resources

An experimental and model-development program was conducted to determine the dispersal characteristics of carbon monoxide emissions from vehicles and the characteristics of wind flows in New York City street canyons. The experimental program involved the measurement of carbon monoxide concentrations and wind conditions on rooftops and at street levels along with traffic flow for several weeks at 7 sites of differing geometries. Continuous monitoring was performed at both street (north-south) and avenue (east-west) sites in Manhattan. The model-development program involved the derivation of an analytic expression to calculate carbon monoxide concentrations and an analysis involving a stepwise linear regression procedure with both wind and carbon monoxide concentration parameters.

The wind measurements and analysis resulted in the definition of several characteristics of wind fields in these street canyons. Near the surface, the winds channel or focus parallel to the street axis. This channeling is more prevalent on streets that have large building-height (H) to street-width (W) ratios. Also, the average wind direction variance is less at the locations with greater H/W ratios.

The linear stepwise regression analysis reveals that the winds near the surface of the streets, which are 800 ft (244 m) long, are much better correlated to prevailing winds (i.e., the winds measured at the Central Park Weather Station) than those on the avenues, which are only 200 ft (61 m) long. The regression analysis produced equations that accurately predict surface wind on the streets with a residual mean square value of typically 5 $(\text{mph})^2$ [8 $(\text{km/h})^2$].

In general, the surface winds are less than those at rooftop locations, and greater H/W ratios produce higher surface wind speeds. For example, the measurements at one surface site on an avenue surrounded by tall (400-ft or 122-m) buildings showed greater wind speeds than are seen at an avenue site with short (50-ft or 15-m) buildings. The greater H/W ratios also produce a greater correlation between rooftop and surface wind directions. Except for the site with the lowest H/W ratio (0.5), the wind angles between the surface and rooftop positions are within 90 deg of one another 72 to 97 percent of the time. They are not correlated at the site with an H/W ratio of 0.5. Occasionally at the sites with low H/W ratios, there is some evidence that a circulation or helix pattern forms in the canyons for a short time.

One-hour air bag samples were acquired at the surface and analyzed for carbon monoxide concentration to determine the characteristics of concentrations near the street traffic. A 1-way analysis of variance was performed on the air bag samples. This analysis reveals that, at the 5 percent level of significance, there is no discernible difference in the carbon monoxide concentrations measured along the block at least 40 ft (12 m) from the corners and equidistant from the curb at a height of 5 ft (1.5 m). In addition, the variance calculated between the individual air bag concentrations and the mean value of all air bags (filled simultaneously) along the block reveals greater ventilation than at midblock. Also, the concentrations measured at all corners are not necessarily equal to one another. The average difference in carbon monoxide concentration across a 15-ft (1.3-m) sidewalk is approximately 0.97 (s.e. 0.13) ppm.

The analysis of the carbon monoxide concentrations at the various sites reveals that the ratio of the concentration difference between the surface and the rooftop levels (ΔC) and the vehicular emissions (Q) increases with greater H/W ratios. Approximately 40 linear regression analyses involving ΔC as the dependent variable, and products of Q and reciprocals of the Cartesian components of wind were performed.

The model predictions of this ratio for a uniform diffusivity constant agree well with the regression parameters averaged over a wide range of meteorological conditions. The model equation is

$$\frac{\Delta C}{Q} \propto \ell n\left[4\left(\frac{H}{W}\right)^2 + 1\right] + \ell n\left[\frac{4}{9}\left(\frac{H}{W}\right)^2 + 1\right]$$

Furthermore, there is evidence that the effective diffusivity constant is related to the reciprocal of the wind speed.

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PARTICIPANTS AND SPONSORSHIP OF THIS SPECIAL REPORT

Participants

Andrew, Donald, Bureau of Air Quality and Noise Control, Maryland Department of Health, Baltimore
Angus, Richard M., Monitoring and Data Analysis Division, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina
Ashe, Raymond A., Jr., Florida Department of Transportation, Tallahassee

Bell, John Kenneth, Nevada Highway Department, Reno
Blake, Stephen E., Transportation Research Board
Bonta, William K., Bureau of Air Quality and Noise Control, Maryland Department of Health, Baltimore
Brooks, Andrew, Regional Office, Maryland State Highway Administration, Baltimore

Caruso, Salvator, Office of Highway Planning, Federal Highway Administration, Washington, D.C.
Chaves, Jesse R., Office of Environment and Design, Region 3, Federal Highway Administration, Baltimore
Chernisky, John, Federal Highway Administration, Washington, D.C.
Clemeña, Gerry G., Virginia Highway and Transportation Research Council, Charlottesville
Coffey, Peter E., New York Department of Environmental Conservation, Albany
Cook, Kenneth E., Transportation Research Board

Dabberdt, Walter F., Environmental Meteorology Program, Stanford Research Institute, Menlo Park, California
Demerjian, Kenneth L., Atmospheric Modeling and Assessment Branch, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina
Dimitriades, Basil, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina
Donley, Diane, Natural Resources Defense Council, Washington, D.C.
Douglas, Robert, Environmental Branch, City of Baltimore
Downey, Paul J., Transportation Systems Center, U.S. Department of Transportation, Cambridge, Massachusetts

Ellis, George W., Urban Planning Bureau, Alabama Highway Department, Montgomery
Eschenroeder, Alan, Environmental Research and Technology, Inc., Santa Barbara, California
Everett, A. G., American Petroleum Institute, Washington, D.C.

Gastler, John H., Connecticut Department of Transportation, Wethersfield
Guthman, Lewis E., New York City Department of Air Resources

Halvorson, James P., Minnesota Department of Highways, St. Paul

Hamer, Thomas, Environmental Branch, Maryland Department of Transportation, Baltimore
Horowitz, Joel L., Office of Policy Analysis, U.S. Environmental Protection Agency, Washington, D.C.
Hoyles, Michael, Washington State Department of Highways, Olympia
Hunt, James W., Office of Development, Federal Highway Administration, Washington, D.C.

Iwanchuk, Robert, Environmental Research and Technology, Inc., Concord, Massachusetts

Jain, Ashok K., Virginia Air Pollution Control Board, Richmond
Jones, Kenneth E., Office of Research, Federal Highway Administration, Washington, D.C.
Jongedyk, Howard A., Office of Research, Federal Highway Administration, Washington, D.C.

Kerby, E. Gordon, II, Virginia Department of Highways and Transportation, Richmond
Kirschensteiner, James, Federal Highway Administration, Washington, D.C.
Koschek, Kenneth C., New Jersey Department of Environmental Protection, Trenton
Kozlowski, Thomas P., Office of Highway Planning, Federal Highway Administration, Washington, D.C.
Kurtzweg, Jerry A., Land Use Policy Branch, U.S. Environmental Protection Agency, Washington, D.C.

Latshaw, Gary, Environmental Systems Laboratory, Sunnyvale, California
Lawler, Dennis A., Division of Air Pollution Control, Illinois Environmental Protection Agency, Springfield

Marmo, Fred, Transportation Systems Center, U.S. Department of Transportation, Cambridge, Massachusetts
Mason, F. J., Environmental Research Office, Ford Motor Company, Dearborn, Michigan
McCurdy, Thomas, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina
McLean, Brian, Pennsylvania Department of Transportation, Harrisburg
Mellem, Norman, Minnesota Department of Highways, St. Paul

Nash, Carlton T., Virginia Department of Highways and Transportation, Richmond
Noll, Kenneth E., Illinois Institute of Technology, Chicago
Nussbaum, Barry D., U.S. Environmental Protection Agency, Washington, D.C.

Paisie, Joseph, Bureau of Air Quality and Noise Control, Maryland Department of Health, Baltimore
Palmieri, F. L., New York State Department of Transportation, Albany
Papetti, Robert A., Office of Air, Land and Water Use, U.S. Environmental Protection Agency, Washington, D.C.
Patterson, Robert M., Technology Division, GCA Corporation, Bedford, Massachusetts
Piracci, Ronald J., New York State Department of Transportation, Albany
Prasad, Chandrika, Virginia Air Pollution Control Board, Richmond

Ranzieri, Andrew J., California Department of Transportation, Sacramento
Roth, Philip M., Environmental Studies Systems Applications, Inc., San Rafael, California

St. John, James E., Federal Highway Administration, Trenton, New Jersey
Seinfeld, John H., California Institute of Technology, Pasadena
Shirley, Earl C., California Department of Transportation, Sacramento

Sievers, Henry, Texas Air Control Board, Arlington
Sistla, Gopal, New York State Department of Environmental Conservation, Albany
Smith, Wayne, New Jersey Department of Transportation, Trenton
Sokolowski, Henry, Pennsylvania Department of Transportation, Harrisburg
Sontowski, John, Bureau of Technical Services, New York City Department of Air Resources
Stephens, N. Thomas, Department of Civil Engineering, Virginia Polytechnic Institute and State University, Blacksburg

Toth, Gary, New Jersey Department of Transportation, Trenton
Trijonis, John, Technology Service Corporation, Santa Monica, California

Walsh, Michael, Mobile Source Enforcement Division, U.S. Environmental Protection Agency, Washington, D.C.
Wambsgans, D. E., II, District of Columbia Bureau of Air and Water Quality Control, Washington, D.C.
Whitten, Gary, Systems Applications, Inc., San Rafael, California
Williams, Marcia E., Office of Mobile Source Air Pollution Control, U.S. Environmental Protection Agency, Ann Arbor, Michigan
Wilson, Kent R., University of California, San Diego
Wood, Herbert T., Air and Water Quality Monitoring Division, District of Columbia Bureau of Air and Water Quality Control, Washington, D.C.
Worth, James J. B., Research Triangle Institute, Research Triangle Park, North Carolina

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To share in the task of furthering science and engineering and of advising the federal government, the National Academy of Engineering was established on December 5, 1964, under the authority of the act of incorporation of the National Academy of Sciences. Its advisory activities are closely coordinated with those of the National Academy of Sciences, but it is independent and autonomous in its organization and election of members.